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Review Article

Advanced Multifunctional Nanomaterials for Sustainable Energy and Environmental Applications: Green Synthesis, Surface Engineering, Catalysis, Energy Storage, Water Purification, and Chemical Sensing

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Abstract

Advanced multifunctional nanomaterials are emerging as versatile platforms for addressing interconnected energy and environmental challenges through tunable composition, high surface area, engineered interfaces, and nanoscale reactivity. This review critically examines the design, synthesis, functionalization, and application of metal, metal oxide, carbon-based, polymeric, porous, two-dimensional, and hybrid nanomaterials. Particular emphasis is placed on green synthesis, renewable precursors, low-impact fabrication, waste-derived feedstocks, scalability, and life-cycle sustainability. The role of surface functionalization, heteroatom doping, defect engineering, heterostructure formation, and interfacial charge transfer in controlling catalytic, optical, electrochemical, and adsorption properties is systematically discussed. Applications in heterogeneous catalysis, photocatalytic hydrogen production, carbon dioxide conversion, pollutant degradation, rechargeable batteries, supercapacitors, and emerging flexible storage devices are evaluated using structure–property–performance relationships. The review also explores nanomaterial-enabled water purification, membrane separation, antimicrobial treatment, and chemical, electrochemical, optical, and gas sensing, including integrated remediation–sensing platforms for real-time monitoring. Current barriers involving toxicity, agglomeration, instability, poor selectivity, recovery, reproducibility, standardization, and industrial scale-up are identified. Finally, future directions highlight artificial-intelligence-guided discovery, operando characterization, circular material design, self-healing systems, and safe, economical deployment, establishing a unified roadmap for sustainable multifunctional nanotechnology across energy conversion, storage, environmental remediation, and chemical detection under realistic operating conditions and across diverse environmental matrices worldwide.

Keywords: Multifunctional nanomaterials, Green synthesis, Surface engineering, Energy storage, Environmental remediation, Chemical sensing.

1. INTRODUCTION

Nanotechnology has evolved from the size-controlled preparation of isolated nanoparticles into a multidisciplinary platform for engineering materials whose chemical, electronic, optical, magnetic, mechanical, and interfacial properties can be deliberately programmed. Nanomaterials are commonly described as materials possessing at least one structural dimension within approximately 1–100 nm, although contemporary nanoscience also includes hierarchically organized and porous systems whose decisive functions originate from nanoscale domains. This conceptual expansion has

enabled the development of nanoparticles, nanowires, nanotubes, nanosheets, quantum dots, nanofibers, porous frameworks, and hybrid nanocomposites with functions that are not attainable in their bulk counterparts (Jeevanandam *et al.,* 2018; Khan *et al.,* 2019; Baig *et al.,* 2021). Rather than representing merely smaller versions of conventional materials, advanced nanomaterials constitute tunable chemical systems in which atomic arrangement, particle dimensions, morphology, surface termination, porosity, defects, and interfaces collectively determine performance.

The distinctive behavior of nanomaterials arises primarily from the high proportion of atoms located at or near the surface and from size-dependent electronic phenomena. A high surface-to-volume ratio increases the density of accessible adsorption and reaction sites, thereby enhancing catalytic activity, contaminant capture, molecular recognition, and electrochemical interaction. Quantum confinement can modify the density of electronic states, bandgap, photoluminescence, and redox behavior of semiconductor nanocrystals. Metallic nanoparticles may exhibit localized surface plasmon resonance, while nanostructured magnetic materials can display size-dependent magnetic responses useful for separation and recovery. In electrochemical systems, reduced diffusion distances facilitate ion and electron transport, whereas interconnected pores improve electrolyte penetration and mass transfer. These characteristics can be adjusted through controlled synthesis, heteroatom doping, vacancy creation, surface functionalization, and heterostructure construction (Baig *et al.,* 2021; Luo *et al.,* 2019). Consequently, nanoscale engineering provides a direct route for connecting composition and structure with a desired macroscopic function.

The emergence of multifunctional nanomaterials represents a further transition from single-purpose materials to integrated platforms capable of performing two or more complementary tasks. Multifunctionality may arise intrinsically from one material, as in graphene derivatives that combine conductivity, adsorption, mechanical reinforcement, and electrochemical activity, or it may be created by coupling components with different functions. Examples include metal–semiconductor, metal oxide–carbon, polymer–nanoparticle, core–shell, and porous framework-based composites. Within these architectures, the individual components do not simply coexist; electronic coupling, interfacial polarization, strain, defect formation, and complementary mass-transport pathways may generate synergistic behavior. Properly engineered interfaces can promote charge separation in photocatalysts, accelerate redox reactions, stabilize active phases, improve analyte recognition, and suppress structural degradation. Such integration is central to the development of materials that can simultaneously convert energy, store charge, remove contaminants, and detect chemical species. The growing importance of multifunctional nanomaterials is closely linked to the interconnected nature of current energy and environmental challenges. Renewable electricity generation, electrified transportation, distributed electronics, and grid stabilization require storage technologies with greater energy density, power capability, rate performance, lifetime, and safety. Nanostructured electrodes can shorten solid-state diffusion pathways, expose redox-active sites, accommodate mechanical strain, and support flexible device architectures. Accordingly, nanomaterials have become central to research on rechargeable batteries, electrochemical capacitors, and hybrid storage systems (Pomerantseva *et al.,* 2019; Simon & Gogotsi, 2020). Nevertheless, nanosizing is not universally beneficial. Excessive surface area can intensify parasitic reactions, phase instability, particle aggregation, and electrolyte decomposition. The most effective designs therefore combine nanoscale activity with mesoscale transport networks, protective interfaces, and mechanically stable architectures.

Nanomaterials are equally important for sustainable energy conversion. Semiconductor nanostructures, plasmonic particles, single-site catalysts, and conductive hybrids can harvest light, activate small molecules, and lower reaction barriers in photocatalytic and electrocatalytic processes. Applications include hydrogen evolution, oxygen evolution, carbon dioxide reduction, nitrogen fixation, and solar-fuel production. In photocatalysis, performance depends on light absorption, charge generation, carrier separation, surface migration, and interfacial reaction kinetics. Crystal-phase control, defect engineering, cocatalyst deposition, and heterojunction formation can improve these processes by extending spectral response and reducing electron–hole recombination (Luo *et al.,* 2019). More recent analyses of interfacially engineered metal-oxide nanocomposites further demonstrate that the same design principles can support both pollutant degradation and energy-related reactions, emphasizing the convergence of environmental remediation and renewable-energy generation (Ahmed *et al.,* 2025).

Environmental applications have expanded from passive adsorption to integrated treatment and monitoring. Nanoporous carbons, metal oxides, membranes, magnetic nanoparticles, metal–organic frameworks, and functional nanocomposites can remove heavy metals, dyes, pharmaceuticals, pesticides, pathogens, and other emerging contaminants through adsorption, filtration, catalytic transformation, antimicrobial action, or combinations of these mechanisms. Nanostructured sensors can also translate molecular binding, charge transfer, or optical changes into measurable signals, enabling rapid detection at low analyte concentrations. The possibility of combining capture, degradation, magnetic recovery, and sensing in one platform is particularly attractive for decentralized water treatment and real-time environmental surveillance. However, high removal efficiency in

simplified laboratory solutions does not automatically ensure effectiveness in natural or industrial waters, where competing ions, dissolved organic matter, variable pH, fouling, and complex contaminant mixtures can alter material behavior (Nagar & Pradeep, 2020).

The rapid expansion of this field also requires a more critical understanding of sustainability. Nanomaterials designed to solve environmental problems may themselves create burdens if their manufacture depends on toxic reagents, scarce elements, energy-intensive processing, or poorly recoverable particles. Potential release, transformation, bioaccumulation, and toxicity must therefore be assessed alongside technical performance. Green synthesis, renewable or waste-derived precursors, aqueous processing, catalyst recovery, regeneration, and life-cycle thinking are becoming essential elements of responsible nanomaterial development. Pokrajac et al. (2021) argued that nanotechnology can contribute substantially to global sustainability only when innovation is aligned with safety, governance, scalability, and equitable implementation. Thus, the significance of multifunctional nanomaterials lies not only in their exceptional nanoscale properties but also in their capacity to integrate functions across traditionally separated technological domains. Their future impact will depend on moving beyond isolated performance records toward reproducible structure–property–performance relationships, realistic testing, durability, regeneration, safe-by-design synthesis, and manufacturable architectures. A unified evaluation of green synthesis, surface engineering, catalysis, energy storage, water purification, and chemical sensing is therefore necessary to determine how multifunctional nanomaterials can progress from laboratory concepts to reliable technologies for sustainable energy and environmental protection.

Global energy demand, climate change, freshwater scarcity, industrial pollution, and depletion of critical resources are closely interconnected rather than isolated challenges. Energy generation and storage require substantial quantities of water and raw materials, while water extraction, purification, desalination, distribution, and wastewater treatment consume considerable energy. Conventional energy production also generates greenhouse gases and hazardous pollutants, whereas contaminated water and industrial waste streams frequently contain recoverable metals, nutrients, carbon compounds, and chemical energy. Consequently, sustainable development requires an integrated energy–environment approach in which clean-energy production, pollution control, water security, and resource conservation are addressed within a unified technological framework. Multifunctional nanomaterials are particularly relevant to this transition because their composition, porosity, surface chemistry, electronic structure, and interfaces can be engineered to support several complementary processes within a single material or device (Pokrajac *et al.,* 2021; Rani *et al.,* 2022).

Clean-energy technologies depend heavily on advanced materials capable of efficiently converting, storing, and transporting energy. Nanostructured materials have become central to rechargeable batteries, supercapacitors, fuel cells, hydrogen-production systems, solar cells, and electrocatalytic devices because they provide large electrochemically active areas, short ion-diffusion distances, adjustable electronic structures, and controllable reaction sites. In batteries and supercapacitors, nanoscale electrodes can accelerate ion transport and accommodate structural changes during repeated charge–discharge cycles. However, isolated nanoparticles may suffer from aggregation, excessive interfacial reactions, and chemical instability. Hierarchical architectures that combine nanoparticles, conductive carbon frameworks, porous supports, polymers, or two-dimensional materials are therefore increasingly preferred because they balance nanoscale reactivity with macroscopic stability and transport efficiency (Pomerantseva *et al.,* 2019).

The relationship between energy production and water security is especially evident in hydrogen-generation technologies. Water electrolysis and photoelectrochemical water splitting offer routes for converting renewable electricity or solar radiation into hydrogen, a chemical energy carrier that can be stored and subsequently used without direct carbon emissions at the point of utilization. Multifunctional photoelectrodes must simultaneously absorb light, generate and separate charge carriers, transport electrons and ions, catalyse hydrogen and oxygen evolution, and resist chemical degradation in aqueous environments. Carbon materials, metal oxides, perovskites, metal–organic frameworks, and semiconductor heterostructures have therefore been integrated to combine light harvesting, conductivity, catalytic activity, and structural stability. Rajaitha *et al.,* (2022) emphasized that multifunctionality is essential in photoelectrochemical systems because no single conventional material normally possesses all the optical, electrochemical, catalytic, and durability characteristics required for efficient water splitting. Photocatalysis further demonstrates how one material platform can connect clean-energy conversion with environmental remediation. Semiconductor photocatalysts generate electron–hole pairs under light irradiation, and these charge carriers can drive surface reduction and oxidation reactions. Depending on the catalyst, reaction environment, and surface-active species, the same underlying photochemical principles can support hydrogen evolution, carbon dioxide conversion, nitrogen fixation, organic synthesis, air purification, or degradation of aqueous contaminants. Crystal-lattice modification, defect engineering, cocatalyst deposition, heterojunction construction, and surface functionalization can improve light absorption, suppress

charge recombination, and direct interfacial reactions toward selected products. Thus, photocatalytic materials should not be classified exclusively as either energy materials or environmental materials; they form a shared chemical platform whose function is determined by band structure, interfacial kinetics, reactant adsorption, and reactor configuration (Luo *et al.,* 2019).

Water purification itself is an energy-related challenge. Desalination, advanced oxidation, membrane filtration, aeration, pumping, and disinfection can require substantial energy inputs, particularly when conventional treatment trains are used for highly saline or chemically complex waters. Nano-enabled systems can reduce these demands by increasing permeability, improving contaminant selectivity, enabling sunlight-driven reactions, and limiting membrane fouling. Examples include photocatalytic membranes, adsorptive nanocomposites, antimicrobial coatings, nanostructured membrane bioreactors, and photothermal evaporators. Nanomaterial-incorporated membranes may combine filtration with catalytic degradation or microbial inhibition, potentially reducing chemical cleaning requirements and extending operational life. Nevertheless, their practical value depends on preventing nanoparticle release, maintaining flux under realistic conditions, and demonstrating long-term stability and economic viability (Nagar & Pradeep, 2020; Pervez *et al.,* 2020).

Solar-driven interfacial evaporation is a representative technology at the water–energy interface. Rather than heating an entire water body, photothermal materials localize solar energy at the air–water boundary, where evaporation occurs. This approach can reduce thermal losses and support decentralized desalination or wastewater purification without continuous grid electricity. Metal–organic frameworks are attractive for such systems because their pore structures, chemical functionalities, hydrophilicity, and optical behavior can be adjusted through metal-node selection, linker modification, and composite formation. MOF-based evaporators may also provide salt resistance, pollutant adsorption, antimicrobial activity, or evaporation-driven electricity generation. These combined functions illustrate how material design can transform a passive solar absorber into an integrated platform for clean-water production, contaminant management, and energy harvesting (Zhang *et al.,* 2024). Hydrogels provide another example of a material family that bridges energy and environmental applications. Their hydrated three-dimensional networks can be engineered for ionic conductivity, mechanical flexibility, molecular adsorption, water transport, thermal management, and responsiveness to temperature, pH, light, or electric fields. Accordingly, hydrogel-based materials have been investigated as electrolytes and separators for batteries and supercapacitors, as photothermal evaporators, as adsorbents for contaminated water, and as atmospheric water-harvesting media. The same polymer network may contain conductive nanofillers, catalytic particles, hydrophilic groups, or selective binding sites, enabling simultaneous control of charge transport and water–solute interactions. Guo et al. (2020) demonstrated that the tunable physicochemical characteristics of hydrogels make them valuable platforms for linking energy storage and conversion with sustainable water-resource management.

A more advanced form of integration involves treating wastewater as a source of useful products rather than as a waste requiring disposal. Wastewater can contain chemical energy, thermal energy, nitrogen, phosphorus, metals, organic compounds, and reusable water. Electrochemical, photoelectrochemical, membrane-based, and catalytic processes can therefore be designed to couple pollutant removal with energy generation or resource recovery. For example, photoelectrochemical nitrate conversion can transform a contaminant into ammonia or other nitrogen products while coupling the reaction with water oxidation. Selective nanofiltration membranes can separate micropollutants while retaining or recovering valuable nutrients, and electrochemical–osmotic systems may simultaneously recover water, metals, and electrical energy. These approaches replace the linear model of extraction, use, treatment, and disposal with a circular model centred on separation, transformation, recovery, and reuse (Barrera & Bala Chandran, 2021; Zhao *et al.,* 2021).

At the treatment-plant scale, this circular approach could transform wastewater facilities from energy-consuming units into water-reuse and resource-recovery centres. Anaerobic conversion, microbial electrochemical technologies, salinity-gradient energy recovery, nutrient separation, biogas upgrading, heat recovery, and renewable-energy integration can reduce the carbon intensity of wastewater management. Rani et al. (2022) proposed that a net-zero water sector requires improvements in energy efficiency, greater use of on-site renewable energy, recovery of embedded energy from wastewater, and development of decentralized water–energy systems. Multifunctional materials can support this transition through selective membranes, catalytic electrodes, antifouling surfaces, adsorbents, and sensors that monitor process performance in real time.

Resource conservation must also extend to the materials used in clean-energy and environmental technologies. High technical performance cannot be considered sustainable when material production depends on scarce metals, toxic solvents, energy-intensive processing, or components that cannot be recovered after use. Multifunctional design can reduce material consumption by allowing one platform to perform several operations, such as adsorption, degradation, sensing, and magnetic recovery. Waste-derived carbons, biopolymers, earth-abundant metal oxides, regenerable adsorbents, and recyclable catalyst

supports can further reduce dependence on virgin resources. However, multifunctionality should not be pursued merely by adding more components; each component must provide a defined function without creating unacceptable toxicity, synthesis complexity, or end-of-life burdens. Safe-by-design principles, life-cycle assessment, regeneration testing, and critical-material accounting are therefore necessary for evaluating whether multifunctional nanomaterials deliver genuine environmental benefits (Pokrajac *et al.,* 2021).

Overall, the integration of energy and environmental applications represents a shift from single-function performance toward systems-level sustainability. The most promising multifunctional materials are those that connect renewable-energy capture, electrochemical storage, contaminant removal, clean-water production, chemical sensing, and resource recovery through shared structural and interfacial design principles. Future progress will depend on testing these materials under realistic operating conditions, comparing them through standardized performance indicators, and evaluating energy consumption, durability, toxicity, recovery, and life-cycle impacts together. Such an approach can establish multifunctional nanomaterials as enabling components of circular systems in which energy production supports water treatment, waste streams supply recoverable resources, and environmental protection becomes integrated with technological design.

Multifunctional nanomaterials are defined in this review as engineered materials whose nanoscale dimensions, surface characteristics, internal architecture, or interfacial interactions enable two or more complementary functions within a single platform. These functions may include adsorption, catalysis, photocatalysis, electrical conduction, electrochemical charge storage, molecular recognition, antimicrobial activity, optical response, or magnetic recovery. Although nanomaterials are conventionally associated with structures having at least one dimension between approximately 1 and 100 nm, the present review also includes hierarchical and nanoporous materials whose performance is primarily governed by nanoscale structural features. Multifunctionality may arise intrinsically from one material or through synergistic interactions between two or more components assembled as a composite, heterostructure, core–shell system, or layered architecture (Baig *et al.,* 2021; Pokrajac *et al.,* 2021).

The term *multifunctional* is used here in a strict functional sense and does not merely describe a material containing several chemical components. A genuine multifunctional nanomaterial must demonstrate distinct but interconnected functions or a measurable synergistic effect that exceeds the performance expected from its individual constituents. For example, a magnetic photocatalytic nanocomposite may adsorb pollutants, promote their light-driven degradation, and permit catalyst recovery using an external magnetic field. Similarly, a conductive porous nanocomposite may operate as an energy-storage electrode while providing electrocatalytic or chemical-sensing activity. Such behavior is generally controlled by coordinated relationships among composition, particle size, porosity, surface functional groups, defects, electronic structure, and interfacial charge transfer (Luo *et al.,* 2019; De Silva *et al.,* 2025).

The review covers the major families of advanced nanomaterials relevant to sustainable energy and environmental applications. These include metallic nanoparticles; metal, mixed-metal, and transition-metal oxides; semiconductor nanocrystals; carbon nanotubes; graphene and its derivatives; carbon quantum dots; porous and biomass-derived carbons; polymeric nanoparticles; nanofibers; and hydrogel-based nanocomposites. Particular attention is also given to emerging two-dimensional materials, including MXenes, transition-metal dichalcogenides, graphitic carbon nitride, and layered double hydroxides. These material classes provide diverse combinations of conductivity, catalytic activity, surface reactivity, optical response, ion-transport capability, flexibility, and chemical stability, allowing their properties to be tailored for specific energy or environmental functions (Baig *et al.,* 2021; Pomerantseva *et al.,* 2019).

Porous crystalline materials, particularly metal–organic frameworks and covalent organic frameworks, also fall within the scope because their pore dimensions, chemical functionalities, and internal surface environments can be systematically engineered. Metal–organic frameworks consist of metal ions or clusters coordinated with organic linkers, producing structures with tunable porosity, composition, and functionality. These characteristics support applications in adsorption, molecular separation, catalysis, gas storage, pollutant removal, and energy conversion. Their ability to form functional composites with carbon materials, polymers, semiconductors, and magnetic nanoparticles further increases their relevance to multifunctional systems, although water stability, production cost, and large-scale fabrication remain important limitations (Singh *et al.,* 2024). Hybrid and multicomponent nanocomposites constitute a central focus of the review because they can combine the strengths of different material families while compensating for their individual weaknesses. Carbon–metal, carbon–metal oxide, semiconductor–semiconductor, polymer–inorganic, MOF-derived, and magnetic core–shell systems can generate new electronic states, interfacial electric fields, catalytic sites, or transport pathways. These synergistic interactions may increase conductivity, accelerate ion diffusion, improve charge-carrier separation, enhance contaminant binding, or facilitate material recovery. However, increasing compositional complexity can also reduce reproducibility, complicate mechanism identification,

elevate production costs, and make environmental risk assessment more difficult; therefore, complexity must be justified by demonstrable functional improvement (De Silva *et al.,* 2025; Pomerantseva *et al.,* 2019).

The review places particular emphasis on green synthesis and sustainable fabrication. Relevant approaches include plant-mediated and microbial synthesis, biomolecule-assisted reduction, renewable and waste-derived precursors, aqueous processing, mechanochemistry, microwave-assisted synthesis, sonochemistry, and low-temperature hydrothermal methods. Green synthesis is not treated simply as the use of a biological extract; instead, it is evaluated through precursor renewability, solvent toxicity, reaction temperature, energy consumption, product yield, purification demand, reproducibility, scalability, waste generation, and end-of-life management. Comparative life-cycle assessment has demonstrated that a nominally green preparation route does not automatically produce lower overall environmental impacts, particularly when energy-intensive processing or extensive washing is required (Patiño-Ruiz *et al.,* 2021; Pokrajac *et al.,* 2021).

The application scope is organized around four interconnected areas: catalysis and photocatalysis, electrochemical energy storage, water purification, and chemical sensing. The catalytic discussion includes heterogeneous catalysis, photocatalytic pollutant degradation, hydrogen evolution, water splitting, oxygen evolution, and carbon dioxide conversion where these processes clarify transferable structure–activity relationships. Energy-storage coverage focuses on nanostructured electrodes and interfaces for rechargeable batteries, supercapacitors, and emerging flexible or hybrid storage systems. In these technologies, nanostructuring can shorten ion-diffusion pathways and increase active-site accessibility, but it can also accelerate parasitic reactions, structural instability, and electrolyte decomposition (Luo *et al.,* 2019; Pomerantseva *et al.,* 2019).

Water-purification coverage includes adsorption, ion exchange, membrane filtration, photocatalytic degradation, advanced oxidation, antimicrobial treatment, and magnetic separation. Priority is given to materials capable of removing or transforming heavy metals, dyes, pharmaceuticals, pesticides, antibiotics, microorganisms, and other emerging contaminants. Chemical sensing encompasses electrochemical, optical, colorimetric, fluorescence, plasmonic, and gas-sensing platforms in which nanomaterials act as recognition elements, catalytic amplifiers, adsorptive preconcentrators, or signal transducers. Integrated systems capable of detecting contaminants while simultaneously removing or degrading them are of particular interest because they connect environmental monitoring with active remediation (Darwish *et al.,* 2024; De Silva *et al.,* 2025).

Several boundaries are established to maintain conceptual focus. Biomedical drug delivery, tissue engineering, therapeutic nanomedicine, and diagnostic imaging are excluded unless a material or sensing mechanism has direct relevance to environmental or chemical analysis. Conventional bulk materials are excluded when their reported performance cannot be linked clearly to nanoscale structure, surface chemistry, or interfaces. The review also avoids functioning as an exhaustive catalogue of nanoparticles and instead prioritizes studies that reveal mechanistic relationships, multifunctional behavior, comparative performance, regeneration potential, realistic testing, or sustainability implications. Materials evaluated only under ideal laboratory conditions are interpreted cautiously when stability, recovery, interference, fouling, toxicity, or complex sample matrices have not been examined (Darwish *et al.,* 2024; De Silva *et al.,* 2025). The principal objective is to develop an integrated understanding of how multifunctional nanomaterials can support sustainable energy conversion, energy storage, pollution control, water security, and chemical monitoring. More specifically, the review aims to classify major material families; relate nanoscale composition and architecture to functionality; evaluate green synthesis and scalable fabrication methods; assess the influence of surface modification, doping, defects, and heterointerfaces; compare major energy and environmental applications; and identify barriers to practical implementation. It also seeks to establish whether multifunctionality reduces material and process requirements or merely introduces additional synthesis complexity without proportional technological benefit (Pokrajac *et al.,* 2021).

These objectives are guided by several central research questions. Which nanoscale structural and interfacial features enable one material to perform multiple functions? How do precursor selection and synthesis conditions influence morphology, surface chemistry, reproducibility, and environmental impact? Which engineering strategies most effectively improve adsorption, charge separation, ion transport, catalytic activity, and molecular recognition? Can common design principles be transferred among energy storage, photocatalysis, water purification, and chemical sensing? How should materials be compared when performance is reported using different experimental conditions, metrics, and target substances? Finally, what safety, stability, scalability, economic, and regulatory constraints must be addressed before these systems can move from laboratory demonstrations to practical technologies (Patiño-Ruiz *et al.,* 2021; Pokrajac *et al.,* 2021)?

The article is organized to answer these questions sequentially. Following the introduction, Section 2 classifies the principal nanomaterial families and examines their physicochemical properties and structure–property–performance relationships. Section 3

reviews biological, bio-inspired, chemical, and physical fabrication methods, followed by sustainability, scalability, and life-cycle considerations. Section 4 examines surface functionalization, heteroatom doping, defect engineering, heterostructure formation, interfacial charge transfer, and the analytical techniques used to characterize these features. This progression establishes the material and mechanistic foundation required to interpret subsequent applications.

Section 5 evaluates catalytic and photocatalytic applications in sustainable energy conversion and environmental remediation. Section 6 examines rechargeable batteries, supercapacitors, and emerging energy-storage systems, with attention to performance, degradation, and practical device requirements. Section 7 addresses water purification, environmental sensing, and integrated detection–remediation platforms. Section 8 synthesizes the major findings and evaluates toxicity, agglomeration, durability, regeneration, standardization, cost, scale-up, and commercialization, while highlighting artificial-intelligence-guided discovery, operando characterization, circular material design, and safe-and-sustainable-by-design strategies as future priorities. This organization provides a unified pathway from material fundamentals and sustainable fabrication to functional application and real-world implementation.

2. Classification, Properties, and Design Principles of Multifunctional Nanomaterials

2.1. Major Classes of Advanced Nanomaterials

Advanced multifunctional nanomaterials can be classified according to their chemical composition, dimensionality, structural organization, bonding characteristics, and dominant functional properties. The principal categories include metallic and metal-oxide nanoparticles, carbon-based nanomaterials, quantum dots, metal–organic frameworks, covalent organic frameworks, MXenes, polymeric nanomaterials, and hybrid nanocomposites. Each class possesses a characteristic combination of electronic structure, surface chemistry, porosity, conductivity, optical response, and chemical stability. However, the boundaries between these categories are increasingly blurred because contemporary material design commonly integrates several classes into heterostructures or composites capable of performing multiple energy and environmental functions (Baig *et al.,* 2021; Jeevanandam *et al.,* 2018).

Metallic nanoparticles constitute one of the most established classes of functional nanomaterials. Gold, silver, platinum, palladium, copper, nickel, iron, and their alloys display size-dependent catalytic, optical, electrical, magnetic, and antimicrobial properties. Noble-metal nanoparticles are particularly valuable in catalysis and chemical sensing because their surfaces facilitate electron transfer and molecular adsorption, while gold and silver nanoparticles exhibit localized surface plasmon resonance that can enhance optical detection and photocatalytic activity. Platinum- and palladium-based nanoparticles are widely used as electrocatalysts, whereas silver and copper nanoparticles are applied in antimicrobial coatings and water-treatment systems. Nevertheless, high cost, aggregation, surface oxidation, and possible release of toxic metal ions limit the unrestricted application of some metallic nanoparticles (Baig *et al.,* 2021; Jeevanandam *et al.,* 2018).

Metal-oxide nanoparticles include both simple oxides, such as TiO_2, ZnO, Fe_3O_4, CuO, NiO, MnO_2, CeO_2, and SnO_2, and mixed or multimetal oxides, including spinels, perovskites, and layered structures. Their functionality arises from variable oxidation states, semiconductor band structures, oxygen vacancies, acid–base surface sites, and, in some cases, magnetic behavior. TiO_2 and ZnO are extensively investigated as photocatalysts, Fe_3O_4 supports magnetic separation and catalyst recovery, and transition-metal oxides provide reversible redox activity for batteries and supercapacitors. Defect creation, cation substitution, morphology control, and coupling with conductive materials can improve their visible-light absorption, charge transport, catalytic activity, and electrochemical stability. However, poor intrinsic conductivity, particle agglomeration, photocorrosion, and rapid electron–hole recombination frequently necessitate further surface or interface engineering (Luo *et al.,* 2019; Baig *et al.,* 2021). Carbon-based nanomaterials comprise carbon nanotubes, graphene, graphene oxide, reduced graphene oxide, fullerenes, carbon nanofibers, carbon quantum dots, porous carbons, activated carbons, and biomass-derived carbon structures. Their usefulness originates from carbon's diverse bonding configurations, which permit the formation of zero-, one-, two-, and three-dimensional architectures with tunable electrical, mechanical, surface, and adsorption properties. Carbon nanotubes combine high aspect ratio, electrical conductivity, mechanical strength, and accessible internal and external surfaces, whereas graphene-based materials provide two-dimensional conductive networks and chemically modifiable oxygen-containing groups. Porous and heteroatom-doped carbons offer high surface area and adjustable pore-size distributions, making them suitable for adsorption, electrocatalysis, gas capture, batteries, supercapacitors, membranes, and sensors (Hughes *et al.,* 2024; Pomerantseva *et al.,* 2019).

Carbon materials are also advantageous as supports for metals, metal oxides, semiconductors, and polymers because they can reduce nanoparticle aggregation and facilitate charge transport. Nitrogen, sulfur, phosphorus, and boron doping can redistribute electron density and create chemically active sites without requiring large quantities of precious metals. Nevertheless, carbon nanomaterials are not intrinsically sustainable; their environmental value depends on precursor origin, synthesis temperature, purification requirements, dispersibility, recovery, and potential

biological effects. Conventional carbon nanotube and graphene production may require high temperatures or harsh reagents, whereas waste-derived porous carbons and carbon dots offer promising alternatives when their synthesis is designed according to green-chemistry and life-cycle principles (Hughes *et al.,* 2024; Pokrajac *et al.,* 2021).

Quantum dots are zero-dimensional semiconductor nanocrystals, generally several nanometres in diameter, in which the spatial confinement of charge carriers creates discrete energy levels and size-dependent optical and electronic properties. Their absorption and emission wavelengths can be adjusted through particle size, composition, shape, doping, and core–shell construction. Classical quantum dots include CdSe, CdS, PbS, and related semiconductor systems, while less toxic alternatives include InP, Zn-based nanocrystals, silicon quantum dots, carbon dots, and graphene quantum dots. Their strong light absorption, narrow and tunable emission, photostability, and sensitivity to surface interactions support applications in solar cells, light-emitting devices, photocatalysis, fluorescence sensing, and environmental monitoring (Efros & Brus, 2021).

The functionality of quantum dots is strongly influenced by their surface ligands and defect states because a substantial fraction of their atoms are located at or near the surface. Ligands stabilize colloidal dispersions and control solubility, interparticle spacing, charge transport, and analyte recognition, but long insulating ligands may restrict electronic conductivity. Core–shell structures can passivate surface traps and improve optical stability, while heteroatom doping can introduce additional electronic or magnetic behavior. Despite these advantages, the toxicity of cadmium-, lead-, or other heavy-metal-containing quantum dots remains an important concern. The development of heavy-metal-free compositions, greener synthesis, robust encapsulation, and improved end-of-life management is therefore essential for their sustainable application (Efros & Brus, 2021). Metal–organic frameworks are crystalline porous materials constructed from metal ions or metal-containing clusters connected by organic ligands. Their modular architecture allows the independent adjustment of metal nodes, linkers, pore dimensions, surface functionality, and framework topology. MOFs can exhibit exceptionally high internal surface areas and chemically defined adsorption sites, supporting gas storage, carbon capture, molecular separation, pollutant adsorption, catalysis, photocatalysis, chemical sensing, and energy storage. Functional groups introduced through linker selection or post-synthetic modification can improve selectivity toward specific ions or molecules, while incorporation of catalytic metals or photoactive ligands can produce multiple functions within the same framework (Singh *et al.,* 2024).

The major limitations of MOFs include moisture sensitivity, relatively low conductivity, mechanical fragility, and the frequent use of expensive ligands or hazardous organic solvents. Water-stable frameworks, conductive MOFs, nanoscale MOFs, MOF membranes, and MOF-derived carbons or metal oxides have therefore become important research directions. Thermal conversion of selected MOFs can generate porous carbon–metal composites that retain aspects of the precursor architecture while gaining improved conductivity and structural robustness. The resulting materials are relevant to electrocatalysis, batteries, supercapacitors, adsorption, and sensing, although conversion can reduce the molecular precision that originally distinguished the framework (Singh *et al.,* 2024).

Covalent organic frameworks are porous crystalline polymers formed by linking organic building units through strong covalent bonds. Unlike MOFs, their frameworks generally contain light elements such as carbon, nitrogen, oxygen, boron, and sulfur without requiring metal nodes. Their low density, ordered channels, high porosity, chemically adjustable skeletons, and extended π-conjugation make them attractive for gas separation, pollutant adsorption, membrane filtration, photocatalysis, electrocatalysis, energy storage, and fluorescence sensing. Donor–acceptor building blocks can be incorporated into COFs to improve light harvesting and charge separation, while pore-wall functionalization can enhance affinity for target contaminants or catalytic reactants (Ge *et al.,* 2024).

COFs may be classified according to their dimensionality, topology, building-block geometry, and linkage chemistry, including imine, hydrazone, boronate ester, β-ketoenamine, triazine, and imide linkages. The chemical stability of the linkage strongly affects performance under acidic, alkaline, aqueous, or electrochemical conditions. Although COFs possess substantial design flexibility, their production remains challenged by slow crystallization, incomplete structural characterization, limited processability, and difficulties in large-scale synthesis. Nanosheet formation, interfacial polymerization, linkage stabilization, and composite construction are increasingly used to overcome these limitations and expand their practical application (Ge *et al.,* 2024).

MXenes are a rapidly expanding family of two-dimensional transition-metal carbides, nitrides, and carbonitrides generally obtained by selectively removing atomic layers from layered MAX-phase precursors. Their representative formula is commonly expressed as $M_{n+1}X_nT_x$, where M is an early transition metal, X represents carbon or nitrogen, and T_x denotes surface terminations such as –O, –OH, or –F. MXenes combine metallic conductivity, hydrophilicity, mechanical flexibility, high volumetric capacitance, and tunable surface chemistry. These characteristics support

applications in batteries, supercapacitors, electrocatalysis, electromagnetic shielding, desalination, adsorption, photothermal conversion, and chemical sensing (VahidMohammadi *et al.,* 2021). Surface terminations and interlayer spacing govern ion diffusion, molecular adsorption, and electronic behavior in MXenes. Their layered structure can accommodate ions and provide rapid transport pathways, but sheet restacking reduces accessible surface area, while oxidation can degrade conductivity and long-term stability. Strategies such as interlayer pillaring, polymer insertion, heteroatom doping, surface modification, and coupling with MOFs, metal oxides, or carbon materials are used to preserve accessible channels and introduce complementary functions. In particular, MXene–MOF composites combine the conductivity of MXenes with the porosity and chemical selectivity of MOFs, demonstrating how different nanomaterial classes can be integrated through rational interface design (VahidMohammadi *et al.,* 2021; Yang *et al.,* 2023).

Polymeric nanomaterials include polymer nanoparticles, nanofibers, nanogels, hydrogels, conductive polymers, molecularly imprinted polymers, and polymer-based membranes. Their major advantages are chemical versatility, low density, processability, flexibility, and the ability to incorporate selective functional groups. Conductive polymers such as polyaniline, polypyrrole, and poly(3,4-ethylenedioxythiophene) provide redox activity and electrical conductivity for sensors, supercapacitors, batteries, and electrocatalytic systems. Hydrogels contain interconnected polymer networks capable of retaining large quantities of water while transporting ions and molecules, making them useful as electrolytes, adsorbents, separation media, photothermal evaporators, and flexible device components (Guo *et al.,* 2020).

Polymeric materials can also stabilize inorganic nanoparticles, prevent aggregation, improve dispersion, control analyte diffusion, and provide mechanical support. Their limitations include swelling, ageing, restricted thermal stability, low conductivity in non-conjugated systems, and possible loss of functional components. These weaknesses are frequently addressed by incorporating carbon nanomaterials, metal oxides, MXenes, quantum dots, or porous frameworks. Such integration leads to hybrid nanocomposites, which represent the most structurally diverse and technologically important class of multifunctional materials.

Hybrid nanocomposites combine two or more nanoscale constituents to generate complementary or synergistic properties that are unavailable in the individual components. Common examples include metal–metal oxide, carbon–metal oxide, polymer–nanoparticle, quantum dot–semiconductor, MOF–MXene, COF–carbon, and magnetic core–shell systems. Their effectiveness depends on interfacial compatibility, component distribution, chemical bonding, band alignment, pore connectivity, and mechanical integration. Properly designed interfaces can enhance electron transfer, suppress charge recombination, provide hierarchical transport pathways, increase active-site accessibility, and enable simultaneous adsorption, catalysis, sensing, energy storage, and material recovery (Luo *et al.,* 2019; Yang *et al.,* 2023). However, hybridization does not automatically guarantee multifunctionality or superior performance. Excessive compositional complexity may obstruct active sites, increase transport resistance, complicate reproducibility, and create additional environmental or economic burdens. The selection of each component must therefore be linked to a defined function, and synergistic effects should be demonstrated through appropriate controls and mechanistic characterization. The classification of advanced nanomaterials ultimately provides a foundation for understanding their distinctive properties, but future development will increasingly depend on integrating these classes through deliberate surface, defect, pore, and interface engineering rather than treating them as isolated material families.

2.2. Structural, Physicochemical, and Functional Properties

The performance of multifunctional nanomaterials is determined by the interdependence of their structural, physicochemical, and functional properties rather than by chemical composition alone. Particle size, morphology, crystallographic structure, porosity, surface area, electronic band structure, conductivity, mechanical integrity, optical response, and chemical reactivity collectively regulate how a nanomaterial interacts with photons, ions, molecules, electrodes, and surrounding media. As illustrated in Figure 1, reducing particle size, exposing preferential crystal planes, producing defined nanoscale shapes, and introducing surface defects can substantially modify the number and energetic character of accessible active sites. Rational nanomaterial design therefore requires simultaneous control of several properties instead of optimizing a single parameter in isolation (Baig *et al.,* 2021; Gonzalez-Gallardo *et al.,* 2022).

Particle size is among the most influential structural variables because it determines the surface-to-volume ratio and the proportion of under-coordinated atoms located at edges, corners, and external surfaces. As particle dimensions decrease, a larger fraction of atoms becomes accessible for adsorption, electron transfer, redox reactions, and molecular recognition. This effect can increase catalytic activity, sensing sensitivity, ion-storage capacity, and contaminant-removal efficiency. Smaller particles also shorten electron- and ion-diffusion distances, which can improve reaction kinetics in batteries, supercapacitors, electrocatalysts, and photocatalysts. However, extremely small particles possess high surface energies and may undergo agglomeration, dissolution, oxidation, or unwanted side

reactions, demonstrating that the smallest particle size does not necessarily provide the best functional performance (Baig *et al.,* 2021; Pomerantseva *et al.,* 2019).

Particle-size effects are especially pronounced in semiconductor nanocrystals and quantum dots. When particle dimensions approach or become smaller than the exciton Bohr radius, quantum confinement produces discrete electronic energy levels and changes the effective bandgap. Smaller quantum dots generally exhibit wider bandgaps and shorter-wavelength absorption or emission, whereas larger particles display narrower bandgaps and red-shifted optical responses. This size-dependent tunability enables the design of materials for photocatalysis, solar-energy conversion, fluorescence sensing, and light-emitting technologies without changing their fundamental chemical composition. Nevertheless, surface traps and non-radiative recombination pathways may reduce optical efficiency, requiring surface passivation, ligand engineering, or core–shell construction (Efros & Brus, 2021).

Morphology determines the spatial organization of a nanomaterial and controls the exposure of surfaces, transport pathways, and contact with surrounding phases. Zero-dimensional nanoparticles provide high external surface accessibility, while one-dimensional nanowires, nanotubes, and nanofibers support directional charge transport and mechanically connected networks. Two-dimensional nanosheets offer short through-plane diffusion distances and large exposed basal surfaces, whereas three-dimensional flowers, dendrites, aerogels, and hierarchical frameworks integrate surface accessibility with interconnected channels. The nanocubes, nanobars, nanowires, nanofibers, and dendritic structures represented in Figure 1 demonstrate how shape selection can alter active-site density, electron movement, analyte diffusion, and interfacial contact. Morphological engineering is therefore essential for balancing high reactivity with efficient mass transport and structural stability (Gonzalez-Gallardo *et al.,* 2022).

Crystallinity and crystallographic-facet exposure further influence nanomaterial functionality. Highly crystalline structures generally provide continuous pathways for electronic transport and may contain fewer charge-trapping grain boundaries than poorly ordered materials. In contrast, partially amorphous or defect-rich structures may present a greater density of chemically active sites and flexible ion-storage environments. Thus, the optimal degree of crystallinity depends on the required function. Moreover, different crystal facets possess distinct atomic arrangements, coordination environments, surface energies, and adsorption preferences. Preferential exposure of planes such as {111}, {100}, or {110} can consequently alter reaction intermediates, catalytic selectivity, surface oxidation, and molecular binding, as indicated by the facet-dependent diffraction patterns shown in Figure X (Luo *et al.,* 2019; Gonzalez-Gallardo *et al.,* 2022).

Crystal defects including vacancies, dislocations, grain boundaries, steps, terraces, kinks, and adatoms should not be regarded solely as structural imperfections. Controlled defects can create localized electronic states, expose under-coordinated atoms, improve reactant adsorption, and modify activation barriers. Oxygen vacancies in metal oxides, for example, can alter carrier concentration and visible-light absorption, while edge defects in carbon or two-dimensional materials can generate active sites for catalysis and sensing. Nanoislands and stepped or terraced surfaces, as depicted in Figure 1, provide heterogeneous binding environments that may increase surface reactivity. Excessive defect density, however, can promote carrier recombination, corrosion, mechanical weakening, or uncontrolled side reactions; defect engineering must therefore optimize both defect type and concentration (Luo *et al.,* 2019).

Porosity and specific surface area govern the accessibility of internal surfaces and the movement of molecules or ions through a material. Micropores provide strong confinement and high adsorption capacity, mesopores facilitate electrolyte and contaminant transport, and macropores act as rapid diffusion channels and fluid reservoirs. Hierarchical pore systems that combine these length scales can improve adsorption, separation, catalytic conversion, and electrochemical performance by coupling abundant active sites with efficient mass transfer. High-surface-area carbons are particularly important in electrical double-layer capacitors because their accessible internal surfaces support ion accumulation. However, nominal Brunauer–Emmett–Teller surface area alone does not predict performance: pore size, connectivity, wettability, surface chemistry, and accessibility to the target ion or molecule are equally important (Simon & Gogotsi, 2020).

The relationship between surface area and performance is therefore frequently non-linear. Very narrow pores may exclude solvated ions or restrict molecular diffusion, while excessively open pores may reduce volumetric capacity and mechanical strength. Similarly, increasing porosity can improve adsorption and electrolyte infiltration but weaken the load-bearing framework or reduce electrical continuity. Effective multifunctional materials require a balance among surface area, pore volume, pore-size distribution, framework density, and transport resistance. This balance is especially important for porous electrodes, adsorbents, membranes, catalysts, and sensors that must maintain rapid molecular access without losing conductivity or structural stability during repeated operation (Pomerantseva *et al.,* 2019; Simon & Gogotsi, 2020).

Bandgap and electronic structure determine the capacity of semiconductor nanomaterials to absorb light, generate charge carriers, and drive redox reactions. Bandgap engineering may be achieved through size control, doping, vacancy formation, alloying, strain, phase modification, or heterojunction construction. A narrower bandgap can extend absorption into the visible region, but it does not automatically guarantee greater photocatalytic activity because the conduction- and valence-band positions must remain thermodynamically suitable for the desired reduction and oxidation reactions. Furthermore, photogenerated electrons and holes must be separated and transported to surface-active sites before recombination occurs. Consequently, optical absorption, carrier lifetime, band alignment, surface reaction kinetics, and defect concentration must be evaluated together (Luo *et al.,* 2019; Efros & Brus, 2021).

Electrical conductivity is critical in electrodes, electrocatalysts, electrochemical sensors, and photoelectrochemical systems because it governs charge-transfer resistance and electron transport across particles and interfaces. Conductivity may be improved by increasing crystallinity, forming continuous conductive pathways, introducing charge carriers through doping, or integrating poorly conducting active materials with graphene, carbon nanotubes, conductive polymers, or MXenes. MXenes are particularly attractive because they combine metallic conductivity with hydrophilic and chemically tunable surfaces. Nevertheless, restacking, oxidation, weak interlayer interactions, and void formation can reduce their effective conductivity and durability. These limitations illustrate why macroscopic performance depends not only on the intrinsic conductivity of individual nanosheets but also on their orientation, contact resistance, packing density, and interfacial bonding (VahidMohammadi *et al.,* 2021).

Mechanical stability determines whether a nanomaterial can preserve its architecture during fabrication, handling, fluid flow, bending, thermal cycling, and repeated electrochemical operation. Porous and layered materials may exhibit excellent functional properties but undergo cracking, collapse, delamination, or pulverization when subjected to stress or volume change. Interfacial bridging, polymer reinforcement, dense nanosheet alignment, and flexible conductive networks can improve stress transfer and suppress structural failure. Wan et al. (2021), for example, demonstrated that bridging-induced densification reduced structural voids in MXene films and produced a combination of high tensile strength, toughness, electrical conductivity, and electromagnetic-shielding performance. More recent sequential-bridging strategies have further shown that strong interfacial bonding and reduced porosity can produce exceptionally strong MXene assemblies while retaining multifunctionality (Li *et al.,* 2024).

Optical properties arise from interactions among material composition, particle size, shape, electronic structure, defects, and surrounding dielectric environment. Metallic nanoparticles can exhibit localized surface-plasmon resonance, semiconductor quantum dots produce size-dependent fluorescence, and transition-metal oxides may display defect-related absorption or emission. Anisotropic morphologies such as nanorods and nanoplates can exhibit direction-dependent optical responses, while aggregation may shift or broaden absorption bands. These effects support applications in colorimetric detection, fluorescence sensing, surface-enhanced spectroscopy, photothermal conversion, solar-energy harvesting, and photocatalysis. Optical performance must nevertheless be evaluated alongside photostability, charge-carrier dynamics, surface passivation, and resistance to chemical degradation (Efros & Brus, 2021; Baig *et al.,* 2021).

Chemical reactivity represents the integrated outcome of particle size, facet exposure, surface energy, defects, porosity, electronic structure, and surface functionalization. Edge atoms, vacancies, terraces, and kinks often bind reactants more strongly than fully coordinated atoms on ideal basal planes. Surface ligands and functional groups can further regulate colloidal stability, wettability, molecular affinity, charge transfer, and catalytic selectivity. However, high chemical reactivity may also accelerate oxidation, dissolution, fouling, or non-selective reactions. The central design challenge is therefore to create nanomaterials with sufficiently active and accessible surfaces while maintaining chemical selectivity, structural integrity, and operational stability. The properties summarized in Figure 1 should consequently be viewed as an interconnected design network in which modification of one parameter can improve one function while compromising another. Successful multifunctional nanomaterials emerge from balancing these relationships for the intended energy, environmental, catalytic, or sensing application (Baig *et al.,* 2021; Pomerantseva *et al.,* 2019).

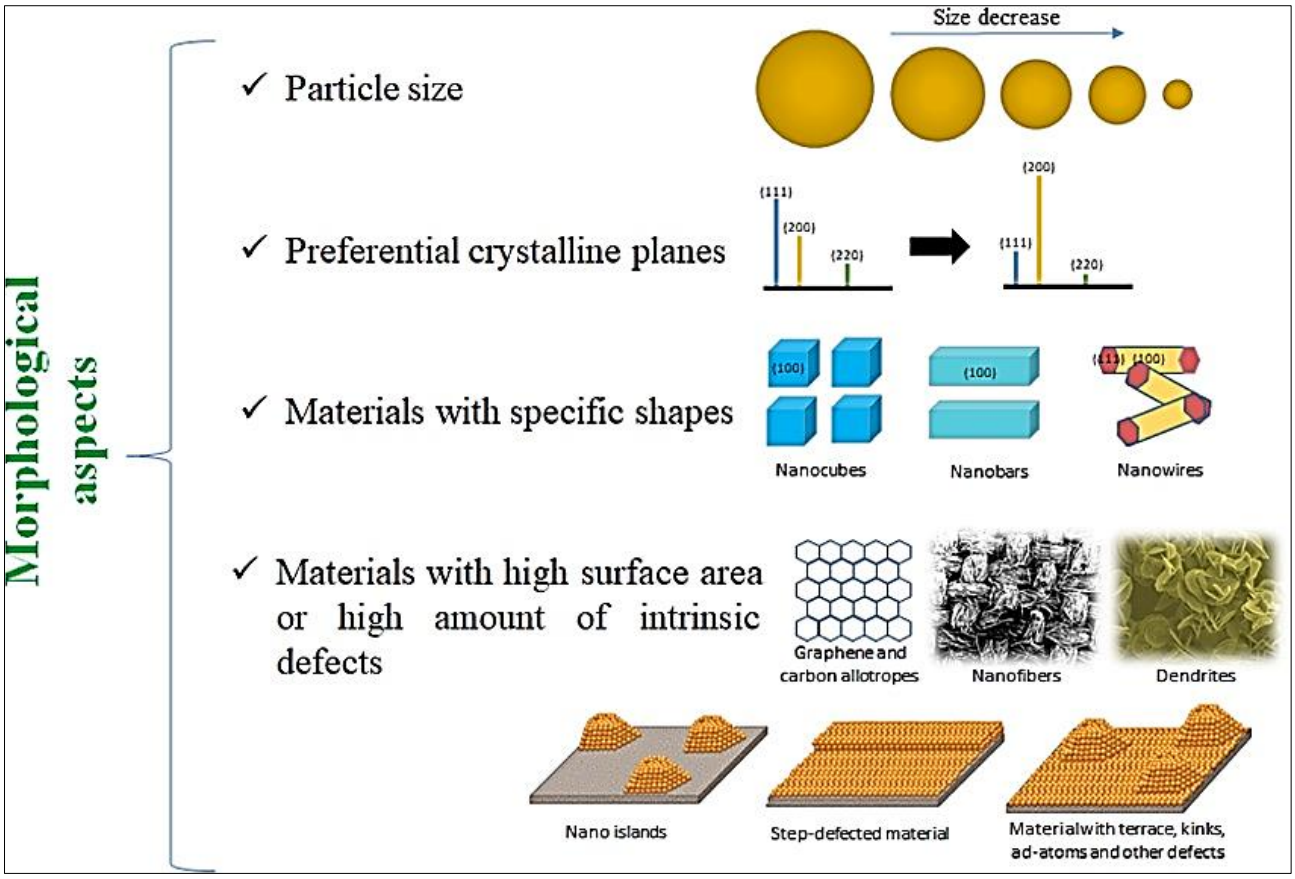

Figure 1: Morphological and Surface-Structural Controls on Nanomaterial Functionality Gonzalez-Gallardo et al. (2022)

The figure illustrates how particle size, exposed crystallographic planes, morphology, high-surface-area architectures, and surface defects can be deliberately engineered. These structural variables influence active-site availability, surface energy, adsorption, charge transfer, conductivity, optical behaviour, and chemical reactivity, thereby controlling the functional performance of nanomaterials.

2.3. **Structure Property Performance Relationships**

The functional performance of advanced nanomaterials arises from interconnected relationships among chemical composition, dimensionality, atomic defects, heterostructure architecture, surface-active sites, and interfacial interactions. These variables control electronic structure, charge distribution, adsorption strength, ion and molecular transport, catalytic kinetics, and structural stability. Figure 2 illustrates this relationship through representative MoS_2-based systems in which edge sites, basal-plane defects, heterointerfaces, and vacancy configurations alter hydrogen adsorption and charge-transfer behavior. The corresponding free-energy profiles emphasize that performance depends not simply on the number of active sites, but also on their atomic configuration and binding energetics (Wang *et al.,* 2023).

Chemical composition determines the electronic orbitals, oxidation states, coordination environments, and bonding characteristics available within a nanomaterial. In multimetallic systems, each element may contribute a different function, such as modifying electrical conductivity, stabilizing a structural phase, regulating intermediate adsorption, or facilitating a specific reaction step. Composition therefore influences both the identity of active sites and their surrounding electronic environment. However, increasing the number of constituent elements does not automatically improve performance. The spatial distribution, oxidation state, and local coordination of each component must be controlled to prevent inactive phases, elemental segregation, or unfavorable adsorption behavior (Baek *et al.,* 2023).

High-entropy oxides demonstrate how compositional complexity can generate broad distributions of chemically distinct surface sites. Baek et al. (2023) examined spinel-type high-entropy oxides containing five transition-metal cations and found that elemental mixing produced local strain around metal–oxygen bonds. This mixing-induced strain modified the adsorption energies of oxygen-evolution intermediates, while surface composition and coverage further influenced catalytic activity. The study demonstrated that the performance of compositionally complex

materials cannot be interpreted using average bulk composition alone, because chemically and structurally distinct local environments may display substantially different reaction energetics (Baek *et al.,* 2023).

Dimensionality establishes the geometric framework through which active-site exposure, electron transport, molecular diffusion, and mechanical integration occur. Zero-dimensional nanoparticles provide a high fraction of surface atoms, but they may aggregate and develop large interparticle resistance. One-dimensional nanowires and nanorods provide directional pathways for electron transport, while two-dimensional nanosheets expose broad surfaces and minimize through-plane diffusion distances. Three-dimensional porous frameworks can integrate lower-dimensional components into mechanically connected structures with continuous pathways for mass and charge transfer. The optimal dimensionality consequently depends on whether surface accessibility, directional conductivity, pore connectivity, or structural robustness is the dominant requirement.

Hierarchical structures can combine these dimensional advantages within one multifunctional architecture. Zhai *et al.,* (2020) constructed two-dimensional MoO_x/MoS_2 nanosheets on one-dimensional NiO_x/Ni_3S_2 nanorods supported by a three-dimensional conductive framework. This arrangement increased interfacial contact, exposed electrochemically accessible sites, and created continuous transport pathways. The resulting $NiMoO_x$/NiMoS structure displayed lower charge-transfer resistance and stronger bifunctional activity than the individual or less complex components. These findings illustrate that dimensional integration can improve performance when each structural level performs a defined role rather than merely increasing morphological complexity (Zhai *et al.,* 2020). Atomic defects provide another direct link between structure and function. Vacancies, interstitial atoms, antisite defects, grain boundaries, dislocations, and edge terminations disrupt periodic bonding and create local electronic states. These sites may change carrier density, expose coordinatively unsaturated atoms, strengthen molecular adsorption, or lower activation barriers. In two-dimensional transition-metal dichalcogenides, the basal plane is often less reactive than under-coordinated edge sites. Introducing controlled defects can activate this otherwise inert area and substantially increase the fraction of the material that participates in surface reactions (Wang *et al.,* 2023; Xu *et al.,* 2022).

Xu et al. (2022) demonstrated this principle using Frenkel-defected monolayer MoS_2, in which molybdenum atoms moved from their lattice positions to nearby interstitial sites, simultaneously creating vacancies and interstitial defects. This atomic rearrangement redistributed surface charge and produced interstitial Mo sites with more favorable hydrogen adsorption. The optimized defective material required an overpotential of 164 mV at 10 mA cm^{-2}, compared with 358 mV for pristine monolayer MoS_2. This comparison shows that defect identity and configuration can be more important than defect quantity alone, because different defects produce distinct coordination structures and electronic states (Xu *et al.,* 2022).

Defect concentration must nevertheless be optimized carefully. A low defect density may be insufficient to create a meaningful population of active sites, whereas excessive vacancies can disrupt conductive pathways, increase surface energy, accelerate oxidation, or weaken structural stability. In MoS_2, sulfur vacancies create defect states that facilitate hydrogen adsorption, but high vacancy concentrations may destabilize the lattice. The free-energy relationships represented in Figure 2 therefore indicate an optimization problem rather than a simple linear correlation. Defect engineering must identify a concentration and configuration that provide favorable adsorption without producing excessive structural or electronic disorder (Ling *et al.,* 2019; Wang *et al.,* 2023). Hetero structure formation provides a complementary strategy for modifying defective sites without requiring extreme defect concentrations. When two materials are placed in intimate contact, differences in work function, Fermi level, electronegativity, lattice structure, and surface termination can cause interfacial charge redistribution. The resulting electric field, orbital hybridization, or strain may shift electronic states and alter the binding of reaction intermediates. Hetero structures can also combine a highly active but poorly conducting phase with a conductive support, or couple an efficient adsorbent with a catalytic component. Their performance therefore depends strongly on interface quality, contact area, lattice compatibility, and chemical bonding.

Using first-principles calculations, Ling et al. (2019) showed that van der Waals heterostructures could regulate the electronic properties of sulfur vacancies in MoS_2. Coupling defective MoS_2 with functionalized MXenes changed interfacial charge transfer and the energy of defect-related electronic states. In the MoS_2/Ti_2C-OH system, nearly optimal hydrogen adsorption was predicted at a sulfur-vacancy concentration of approximately 2.5 percent, whereas freestanding MoS_2 required a substantially higher vacancy concentration. This result demonstrates that defect and interface engineering can operate cooperatively, allowing the activity of a defect site to be adjusted through its electronic environment rather than through defect multiplication alone (Ling *et al.,* 2019).

The nature and accessibility of surface-active sites ultimately determine where adsorption, electron transfer, bond activation, and product formation occur. Active sites may consist of exposed crystal edges, vacancies, isolated metal atoms, strained bonds, mixed-

metal coordination environments, or interfaces between two phases. Their activity depends on the local coordination number, oxidation state, electronic density, and interaction with neighboring atoms. A large geometric surface area is therefore not sufficient when the exposed surface contains few intrinsically active sites or when those sites are blocked, unstable, or poorly connected to conductive pathways.

Single-atom catalysts provide a clear example of active-site control at the atomic scale. Zhai et al. (2021) stabilized isolated ruthenium atoms on defective NiFe layered double-hydroxide nanosheets. Defects helped anchor the Ru atoms, while the Ru–O coordination environment adjusted intermediate adsorption and promoted both hydrogen and oxygen evolution processes. The Ru_1/D-NiFe LDH catalyst showed an overpotential of 18 mV at 10 mA cm^{-2} for hydrogen evolution, while the complete two-electrode system reached 500 mA cm^{-2} at 1.72 V. The study linked performance to the combined influence of atomically dispersed Ru, defective support sites, accessible two-dimensional surfaces, and accelerated interfacial charge transfer (Zhai *et al.,* 2021).

Synergistic interactions occur when combined structural or chemical features produce a performance improvement greater than that expected from their separate contributions. Such synergy may arise when one component supplies active sites, another improves conductivity, a defect stabilizes an isolated atom, and an interface modifies adsorption energetics. In the hierarchical $NiMoO_x$/NiMoS system, composition, defect formation, dimensional architecture, and heterointerface construction operated simultaneously. Density-functional calculations associated the enhanced performance with optimized adsorption energies, while electrochemical measurements indicated improved charge transfer and accessible active area (Zhai *et al.,* 2020).

However, the term synergy should be used only when supported by appropriate evidence. Performance improvement in a composite may result simply from increased surface area, greater catalyst loading, or better electrical contact rather than a genuine interfacial electronic effect. Reliable structure–property–performance analysis therefore requires comparison with individual components, physically mixed controls, defect-free references, and materials with different interface densities. Microscopy, X-ray photoelectron spectroscopy, X-ray absorption spectroscopy, electrochemical impedance analysis, adsorption-energy calculations, and active-area normalization can collectively distinguish intrinsic site activity from geometric or loading effects (Zhai *et al.,* 2021; Xu *et al.,* 2022).

The structure–property–performance framework is transferable across multifunctional applications. Composition and surface coordination control chemical affinity and catalytic selectivity; dimensionality and porosity regulate transport and accessible area; defects modify band structure and reactivity; and heterointerfaces facilitate charge separation or electron conduction. These effects influence electrocatalysis, photocatalysis, electrochemical storage, adsorption, and chemical sensing, although the optimum structural configuration differs among applications. Highly reactive defect sites may benefit catalysis but accelerate degradation during cycling, while dense interfaces may improve charge transfer but reduce pore accessibility. Rational design must therefore balance activity, selectivity, transport, stability, and recoverability rather than maximizing one property independently. Overall, multifunctional performance emerges from coordinated control across atomic, nanoscale, and hierarchical length scales. Composition defines the available chemistry, dimensionality establishes transport architecture, defects create or modify active states, heterostructures regulate interfaces, and surface sites determine direct interactions with reactants or analytes. Figure 2 summarizes these relationships by showing how atomic configurations and heterointerfacial environments reshape adsorption energetics and reaction pathways. Future material design should consequently integrate experimental characterization with computational modeling and controlled reference systems to identify which structural features truly govern performance and which merely correlate with it.

Figure 2 illustrates how material composition, nanoscale dimensionality, vacancy defects, heterostructure formation, and surface-active sites regulate electronic structure, charge redistribution, adsorption energetics, and reaction pathways. Their coordinated interactions produce synergistic improvements in catalytic activity, charge transport, selectivity, stability, and overall multifunctional performance.

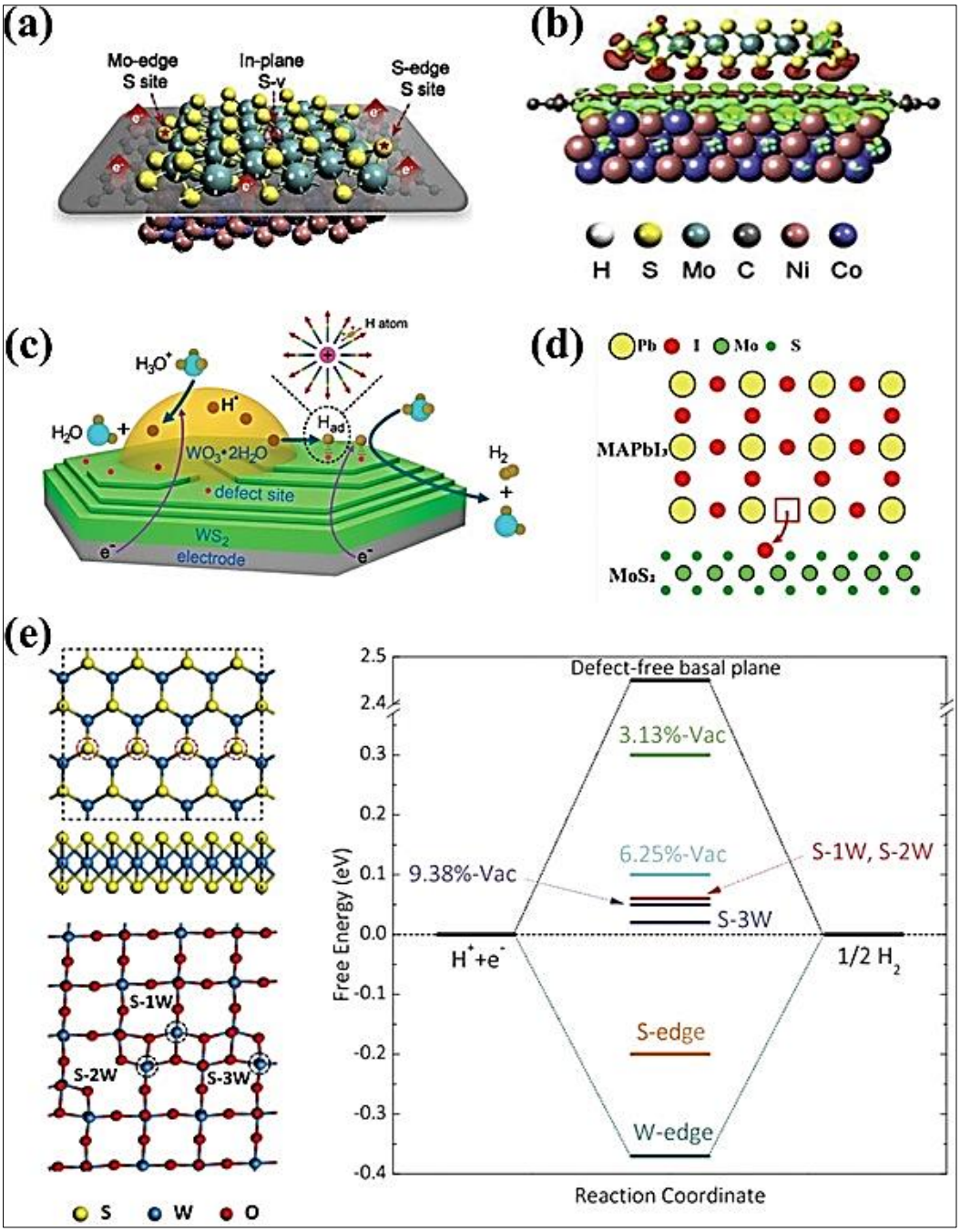

Figure 2: Structure Property Performance Pathways in Multifunctional Nanomaterials: From Dimensionality and Defects to Heterointerface Synergy. Wang *et al.,* (2023)

3. Green Synthesis and Sustainable Fabrication Strategies

3.1. Biological and Bio-Inspired Synthesis Approaches

Biological and bio-inspired synthesis has emerged as an important strategy for producing functional nanomaterials under comparatively mild reaction conditions. Unlike conventional preparation methods that may require strong reducing agents, hazardous stabilizers, organic solvents, high temperatures, or energy-intensive equipment, biological routes use organisms, cellular products, natural extracts, enzymes, proteins, peptides, polysaccharides, and other biomolecules to direct nanoparticle nucleation and growth. These biological components can simultaneously reduce metal ions, stabilize newly formed nuclei, control aggregation, and modify the resulting particle surface. The principal routes include plant-mediated synthesis, microbial synthesis, enzyme-assisted preparation, biomolecule-based reduction, and biomimetic mineralization inspired by natural material-forming processes (Gahlawat & Choudhury, 2019; Tarannum *et al.,* 2019).

Figure 3 summarizes the general workflow of biological nanomaterial fabrication. Plant parts, bacteria, fungi, and algae are processed to obtain extracts, culture filtrates, biomass, or extracellular metabolites containing reducing and stabilizing compounds. When these biological preparations are mixed with appropriate metal precursors, electron-donating biomolecules promote ionic reduction and atomic nucleation, while proteins, polyphenols, sugars, alkaloids, vitamins, and other functional compounds become associated with the developing nanoparticle surface. Differences in biological composition and reaction conditions can consequently produce particles with distinct sizes, morphologies, surface functionalities, catalytic properties, and enzyme-like activities (Huang *et al.,* 2025; Sharma *et al.,* 2022).

Plant-mediated synthesis is among the most widely investigated biological routes because it avoids microbial cultivation and commonly uses accessible leaves, stems, roots, fruits, seeds, bark, flowers, peels, or agricultural residues. Aqueous plant extracts may contain flavonoids, tannins, terpenoids, phenolic acids, alkaloids, reducing sugars, proteins, vitamins, and organic acids. Hydroxyl, carbonyl, carboxyl, and amine groups within these compounds can coordinate precursor ions, transfer electrons, and stabilize nanoparticle surfaces after nucleation. As a result, one extract may perform the combined roles of reducing agent, capping agent, dispersant, and surface-functionalization medium (Tarannum *et al.,* 2019; Sharma *et al.,* 2022).

The plant-mediated process generally involves preparation of an aqueous extract, filtration, addition to a metal-salt solution, and controlled incubation until nanoparticle formation occurs. Reaction variables such as plant species, tissue type, extraction solvent, extract-to-precursor ratio, metal-ion concentration, temperature, pH, mixing rate, light exposure, and reaction time influence nucleation and growth. Alkaline conditions may increase the ionization and reducing capacity of phenolic compounds, whereas elevated temperatures can accelerate reduction but may also degrade heat-sensitive biomolecules. Plant synthesis is therefore operationally simple, but its reproducibility depends on the chemical consistency of the biological source and careful standardization of extraction and reaction parameters (Sharma *et al.,* 2022; Huang *et al.,* 2025).

Microbial synthesis uses bacteria, fungi, yeasts, actinomycetes, and algae either as living nanofactories or as sources of cell-free metabolites. Microorganisms naturally interact with metal ions through detoxification, sequestration, reduction, precipitation, and biomineralization processes. Nanoparticles may form intracellularly following metal uptake and enzymatic reduction, on cell walls through adsorption and nucleation, or extracellularly through secreted reductases, proteins, quinones, peptides, and exopolysaccharides. Extracellular synthesis is generally more convenient for product recovery because the particles can be separated from culture supernatants without disrupting cells or removing large quantities of intracellular material (Gahlawat & Choudhury, 2019).

Bacteria provide rapid growth, genetic manipulability, and diverse metal-resistance mechanisms, making them promising for controlled biosynthesis. Enzymes associated with electron-transfer pathways, particularly reductases using NADH or NADPH as electron donors, can convert dissolved metal ions into lower-valence or elemental forms. Extracellular polysaccharides and proteins can then prevent uncontrolled aggregation through steric and electrostatic stabilization. Bacterial synthesis has been demonstrated for metals and metal-containing materials such as silver, gold, palladium, platinum, copper, iron oxides, zinc oxide, and semiconductor nanocrystals, although particle recovery, sterile operation, and sensitivity to culture conditions remain important practical considerations (Gahlawat & Choudhury, 2019).

Fungi offer several advantages over bacterial systems, including tolerance to relatively high metal concentrations, production of abundant biomass, secretion of substantial quantities of extracellular proteins and enzymes, and comparatively straightforward separation of fungal biomass from liquid media. Fungal filtrates may contain reductases, peptides, quinones, amino acids, and other metabolites that participate in precursor reduction and particle stabilization. Furthermore, the biological corona formed during mycosynthesis can enhance colloidal stability and introduce functional surface groups. Nevertheless, fungal strain, cultivation time, nutrient composition, biomass quantity, pH, temperature, and precursor concentration strongly affect particle size, surface charge, and morphology (Guilger-Casagrande & de Lima, 2019).

Algae and photosynthetic microorganisms provide another renewable platform for biological synthesis. Macroalgae and microalgae contain polysaccharides, pigments, proteins, polyphenols, fatty acids, and antioxidants capable of reducing and stabilizing nanomaterials. Their high growth rates, ability to use sunlight and carbon dioxide, and compatibility with aquatic cultivation make them attractive for sustainable material production. However, seasonal variations, species-specific biochemical composition, salinity, harvesting requirements, and the need to remove residual biomass can influence process consistency. As Figure 3 indicates, algal extracts can generate surface-functionalized particles, but precise control requires characterization of the active biochemical fractions rather than treating the whole extract as an undefined reagent mixture (Gahlawat & Choudhury, 2019; Huang *et al.,* 2025).

Enzyme-assisted synthesis represents a more chemically defined alternative to whole-cell and crude-extract methods. Purified oxidoreductases, nitrate reductases, hydrogenases, and related enzymes can catalyse metal-ion reduction through controlled electron-transfer reactions. Enzymes may also serve as molecular templates that confine nucleation, regulate crystal growth, or stabilize particle surfaces. Compared with crude biological preparations, purified enzymes can improve mechanistic understanding and batch reproducibility. Their disadvantages include production cost, restricted operating ranges, loss of activity, dependence on cofactors, and the need for recovery or immobilization if repeated use is required (Gahlawat & Choudhury, 2019; Vigil & Spangler, 2024).

Biomolecule-based reduction extends this approach to isolated proteins, peptides, amino acids, vitamins, sugars, polysaccharides, and plant-derived phenolics. Molecules such as ascorbic acid, glucose, chitosan, alginate, cellulose derivatives, lignin, and polyphenols can donate electrons or bind to growing crystal surfaces. Protein and peptide sequences may exhibit selective affinity toward particular metals or crystallographic planes, allowing them to control nucleation rate, morphology, crystal orientation, and colloidal stability. The resulting organic coating can also introduce hydrophilicity, analyte-binding groups, catalytic microenvironments, or compatibility with polymer and membrane systems (Tarannum *et al.,* 2019; Vigil & Spangler, 2024).

Biomimetic fabrication moves beyond the direct use of natural extracts by reproducing principles observed in biomineralization. Living organisms produce structurally organized materials such as bones, shells, silica structures, and magnetosomes through spatial confinement, molecular recognition, organic templates, and controlled ion transport. Synthetic proteins, peptides, peptoids, nucleic acids, vesicles, and supramolecular assemblies can imitate these processes and guide nanocrystal formation under aqueous and near-ambient conditions. Biomimetic approaches offer greater structural programmability than crude extracts because the sequence, charge, conformation, and binding motifs of the template can be deliberately designed (Rawlings *et al.,* 2019; Vigil & Spangler, 2024).

Rawlings et al. (2019), for example, engineered soluble coiled-coil proteins containing active loops derived from magnetosome-associated proteins. The artificial proteins retained the capacity to regulate magnetite nanoparticle formation while avoiding the aggregation and solubility problems associated with the native membrane proteins. This work demonstrates how biological knowledge can be translated into engineered molecular tools that control inorganic crystallization. Biomimetic mineralization has similarly been used to produce semiconductor nanocrystals and quantum dots by templating crystal growth or catalysing precursor conversion within proteins and other confined biological environments (Rawlings *et al.,* 2019; Vigil & Spangler, 2024). Bio-inspired synthesis is also relevant to multifunctional materials because residual biomolecules can modify surface chemistry and contribute additional activity. A biogenic coating may improve aqueous dispersibility, provide antioxidant or antimicrobial functions, facilitate adhesion to polymers, or create recognition sites for sensing. In nanozymes, material composition and surface-active sites are engineered to reproduce oxidase-, peroxidase-, catalase-, or superoxide-dismutase-like behavior. Figure 3 therefore connects biological synthesis with biomimetic functionality by showing that biogenic extracts influence both particle morphology and the formation of functionalized catalytic surfaces (Huang *et al.,* 2025).

Despite their advantages, biological synthesis methods should not automatically be classified as environmentally sustainable. Cultivation media, sterilization, heating, extraction, centrifugation, repeated washing, freeze-drying, solvent use, and low product yield can contribute substantial energy and material burdens. Crude extracts may vary with geography, season, genotype, maturity, storage, and extraction protocol, leading to inconsistent particle properties. Moreover, natural capping layers can contain unidentified compounds that complicate toxicity analysis, surface characterization, and regulatory approval. Comparative life-cycle assessment is therefore necessary to determine whether a biological route provides a genuine environmental improvement over an optimized chemical process (Patiño-Ruiz *et al.,* 2021). Future progress requires standardization of biological feedstocks, quantitative metabolite profiling, mechanistic identification of reducing and capping agents, and real-time monitoring of nucleation and growth. Cell-free microbial systems, immobilized enzymes, engineered peptides, synthetic biology, continuous-flow bioreactors, and waste-derived biomolecules could improve reproducibility and scalability. Successful biological fabrication must combine mild processing and renewable inputs with controlled morphology, high yield, low downstream-processing demand, stable functionality, and transparent life-cycle performance. Under these conditions, biological and bio-inspired routes can develop from empirical green synthesis into rational and scalable platforms for manufacturing multifunctional nanomaterials for catalysis, energy storage, water treatment, and chemical sensing.

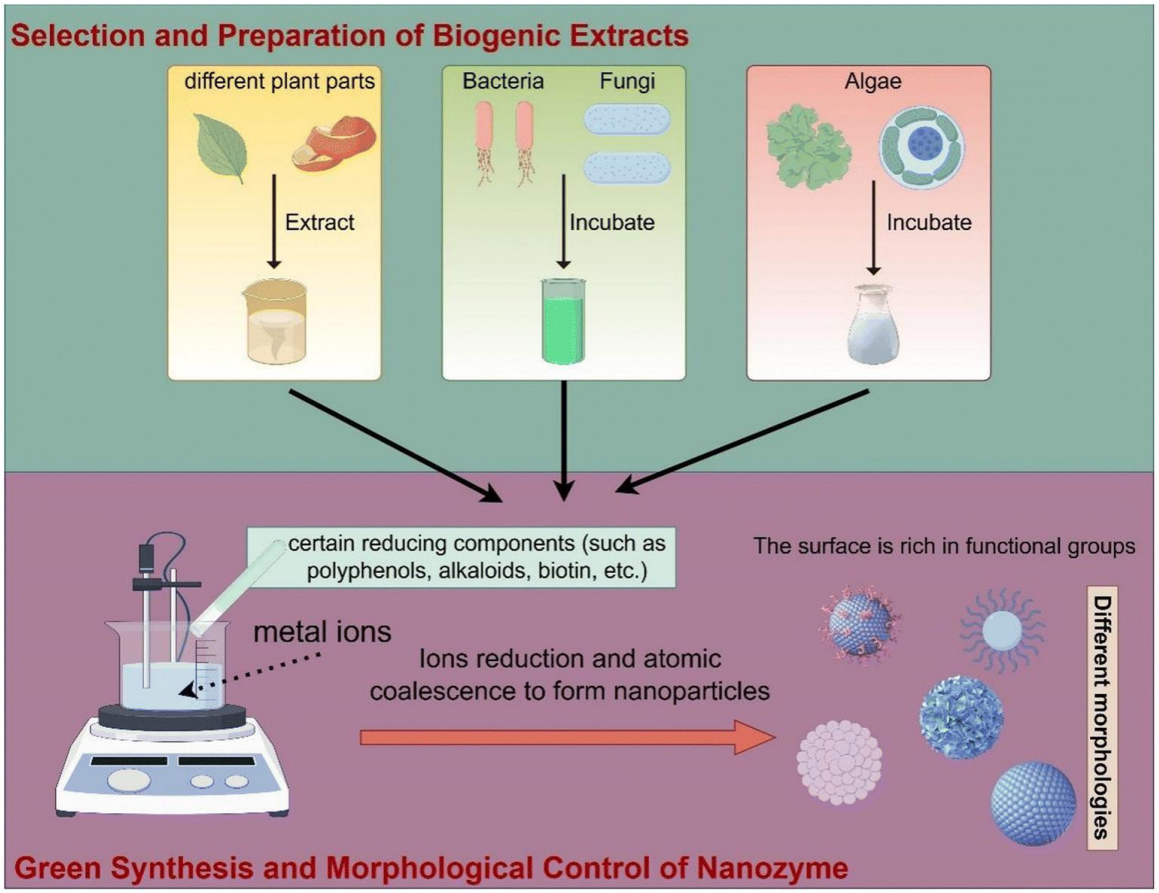

Figure 3: Biological and Bio-Inspired Routes for Sustainable Nanomaterial Fabrication Huang *et al.*, (2025)

Figure 3 illustrates how plant, bacterial, fungal, and algal extracts provide naturally occurring reducing, capping, and stabilizing molecules for converting metal precursors into functional nanomaterials. It also highlights how biological source selection and reaction conditions influence nanoparticle nucleation, morphology, surface chemistry, stability, and enzyme-like functionality.

3.2. Low-Impact Chemical and Physical Fabrication Methods

Low-impact fabrication seeks to reduce the environmental and resource burdens associated with nanomaterial production while preserving control over composition, crystallinity, particle size, morphology, porosity, and surface functionality. Conventional preparation frequently relies on large volumes of organic solvents, prolonged heating, corrosive reagents, repeated purification, or high-temperature calcination. Alternative routes therefore use water-based reaction media, localized energy delivery, mechanical activation, acoustic cavitation, continuous processing, and reduced-temperature crystallization. Figure 4 presents several representative strategies, including hydrothermal, microwave-assisted, mechanochemical, sonochemical, electrochemical, and microfluidic synthesis, illustrating how different energy and mass-transfer mechanisms can direct nanomaterial formation (Lu *et al.,* 2024; Sajini & Joseph, 2025).

Solvent-free and solvent-minimized synthesis is particularly important because solvents may account for a substantial fraction of the material input, waste production, toxicity, and separation requirements of chemical manufacturing. In nanomaterial fabrication, dry solid-state reactions, thermal decomposition without bulk solvents, mechanochemistry, and liquid-assisted grinding can reduce or eliminate conventional reaction media. This approach can increase process mass intensity, simplify product isolation, and minimize solvent recovery. However, a solvent-free label does not automatically establish sustainability because milling energy, precursor hazards, additives, washing steps, and post-synthesis heat treatment must also be considered when evaluating the complete process (Tsuzuki, 2021; Sajini & Joseph, 2025).

Hydrothermal processing uses aqueous precursor solutions in sealed reactors at temperatures above the normal boiling point of water, producing autogenous pressure that promotes hydrolysis, condensation, dissolution, recrystallization, and crystal growth. Water functions as both reaction medium and transport phase, reducing reliance on volatile organic solvents. By adjusting temperature, pressure, pH, precursor concentration, mineralizers, and residence time, hydrothermal synthesis can produce metal oxides, sulfides, phosphates, carbon materials, and porous frameworks with controlled phase composition and

morphology. Its closed reaction environment also supports the formation of metastable phases and well-crystallized nanostructures at temperatures below those commonly required in conventional solid-state reactions (Dias *et al.,* 2020; Jackson *et al.,* 2025).

Despite these advantages, conventional batch hydrothermal processing can require long reaction times, pressure-resistant vessels, slow heating and cooling cycles, and energy-intensive post-treatment. Scale-up may also generate temperature and concentration gradients that alter nucleation and particle growth. Continuous-flow hydrothermal synthesis addresses some of these limitations through rapid precursor mixing, improved heat and mass transfer, shorter residence times, and continuous product collection. Jackson *et al.,* (2025) demonstrated an autonomous continuous-flow hydrothermal reactor that combined inline particle-size measurement with machine-learning optimization to control hematite nanoparticle synthesis. Such systems can reduce batch variability and unnecessary experimental consumption, although their sustainability depends on pressure management, heat recovery, reactor durability, and throughput (Jackson *et al.,* 2025).

Microwave-assisted synthesis provides an alternative to heat transfer from the reactor wall by coupling electromagnetic energy directly with polar molecules and ions. Heating occurs through dipolar polarization and ionic conduction, which can produce rapid and comparatively uniform temperature increases within responsive reaction mixtures. Faster heating and shorter reaction times can increase nucleation rates, narrow particle-size distributions, and reduce undesired crystal growth. Microwave processing has been applied to metals, metal oxides, quantum dots, porous frameworks, carbon dots, and hybrid nanocomposites, commonly in combination with aqueous, hydrothermal, or biological reaction media (Sajini & Joseph, 2025).

The influence of microwave heating was demonstrated by Dias et al. (2020), who compared microwave and conventional hydrothermal routes for SnO nanoparticles. Microwave treatment produced a single tetragonal SnO phase after one hour and yielded spherical particles with an average size of approximately 9 nm. Conventional hydrothermal treatment required four hours to obtain the single phase and generated larger, nonuniform, elongated particles. The difference was attributed mainly to faster and more homogeneous heating, which accelerated precursor conversion and favored rapid nucleation. This comparison shows that the method of energy delivery can determine reaction kinetics, crystallite development, and final morphology even when similar precursor chemistry is employed (Dias *et al.,* 2020).

Microwave processing should nevertheless be evaluated through measured energy consumption rather than reaction time alone. Microwave penetration depends on reactor geometry, sample volume, dielectric properties, and temperature, while nonuniform fields may create local hot regions during scale-up. Some microwave syntheses also retain toxic solvents, surfactants, or energy-demanding purification and calcination stages. The environmental benefit is therefore strongest when rapid microwave heating is combined with water, renewable reagents, concentrated reactions, high product yield, minimal washing, and energy-efficient reactor design. Reporting absorbed power, reaction mass, yield, and total post-processing energy is necessary for meaningful comparison with conventional heating (Sajini & Joseph, 2025).

Sonochemical synthesis uses high-frequency sound waves to generate acoustic cavitation, involving the formation, growth, and rapid collapse of bubbles in a liquid medium. Bubble collapse creates localized physical and chemical effects, including intense microscale heating, pressure pulses, shock waves, microjets, radical formation, surface cleaning, particle fragmentation, and enhanced mixing. These effects can accelerate precursor conversion, initiate nucleation, reduce particle agglomeration, and alter crystal growth. Sonochemistry has therefore been applied to metals, oxides, sulfides, porous materials, composites, and nanosheets, either as the primary synthesis route or as an intensification step during precipitation, crystallization, exfoliation, and surface modification (Devos *et al.,* 2025).

The effectiveness of sonochemical processing depends on frequency, acoustic power, reactor dimensions, probe position, solvent properties, temperature, dissolved gases, and treatment duration. These variables determine the number and intensity of cavitation events and therefore influence nucleation, particle size, porosity, and defect formation. Ultrasound can shorten processing and improve dispersion, but scale-up remains difficult because the acoustic field may become nonuniform in larger reactors. Probe erosion can introduce impurities, while prolonged sonication may consume substantial electricity or damage desired structures. Consequently, ultrasound should be treated as a controllable process-intensification technology rather than being assumed to be inherently green (Devos *et al.,* 2025).

Mechanochemistry uses mechanical forces generated by grinding, compression, impact, or shear to initiate chemical reactions and structural transformations. Ball mills, planetary mills, shaker mills, and extrusion-based systems repeatedly deform and fracture solid reactants, producing fresh surfaces, lattice disorder, intimate mixing, and locally activated reaction sites. Mechanochemical synthesis can operate at or near room temperature and often requires no bulk organic solvent. It has been used to prepare metal oxides, alloys, coordination frameworks, catalysts, doped materials, and nanocomposites. As represented in Figure 4, direct

milling of solid precursors can convert them into porous frameworks without the extended solvent-based crystallization required by conventional methods (Tsuzuki, 2021; Lu *et al.,* 2024).

Mechanochemical performance is governed by milling frequency, time, ball-to-powder ratio, vessel geometry, ball material, atmosphere, precursor hardness, and the relative contributions of impact and shear. Small quantities of liquid may be introduced through liquid-assisted grinding to improve ion mobility and phase selectivity while maintaining far lower solvent consumption than solution synthesis. Important limitations include wear of the milling vessel, contamination from balls, difficulty in measuring local temperature and pressure, and possible formation of amorphous or highly strained products. Some reactions also require subsequent washing or calcination to remove by-products and complete phase development, reducing the overall environmental advantage (Tsuzuki, 2021).

Low-temperature fabrication aims to lower thermal energy demand while preventing particle coarsening, decomposition of sensitive components, and loss of surface functional groups. Suitable strategies include aqueous precipitation, low-temperature hydrothermal processing, electrodeposition, mechanochemistry, photochemical reduction, and low-melting salt media. Lan et al. (2025) reported a molten-salt-assisted route that produced solid-state fluorescent carbon dots at temperatures of 100 to 142 °C within ten minutes. Zinc-ion coordination and confinement within the salt medium lowered the effective reaction barrier and supported high luminescence, demonstrating that low-temperature processing can simultaneously improve energy efficiency, scalability, and functional-property control (Lan *et al.,* 2025).

A genuinely sustainable fabrication route must be assessed as a complete system rather than through a single favorable characteristic. Water-based hydrothermal synthesis may still be energy intensive, microwave synthesis may depend on hazardous reagents, sonochemistry may have poor energy efficiency at scale, and mechanochemistry may require purification or high-temperature conversion. Appropriate evaluation should therefore include solvent toxicity, energy per unit mass of product, reaction time, yield, atom economy, waste generation, water use, material recovery, equipment lifetime, reproducibility, and scale-up potential. The most promising future platforms will integrate low-impact energy delivery with continuous processing, inline characterization, closed-loop optimization, renewable precursors, and recovery of solvents, salts, and unreacted reagents (Jackson *et al.,* 2025; Sajini & Joseph, 2025).

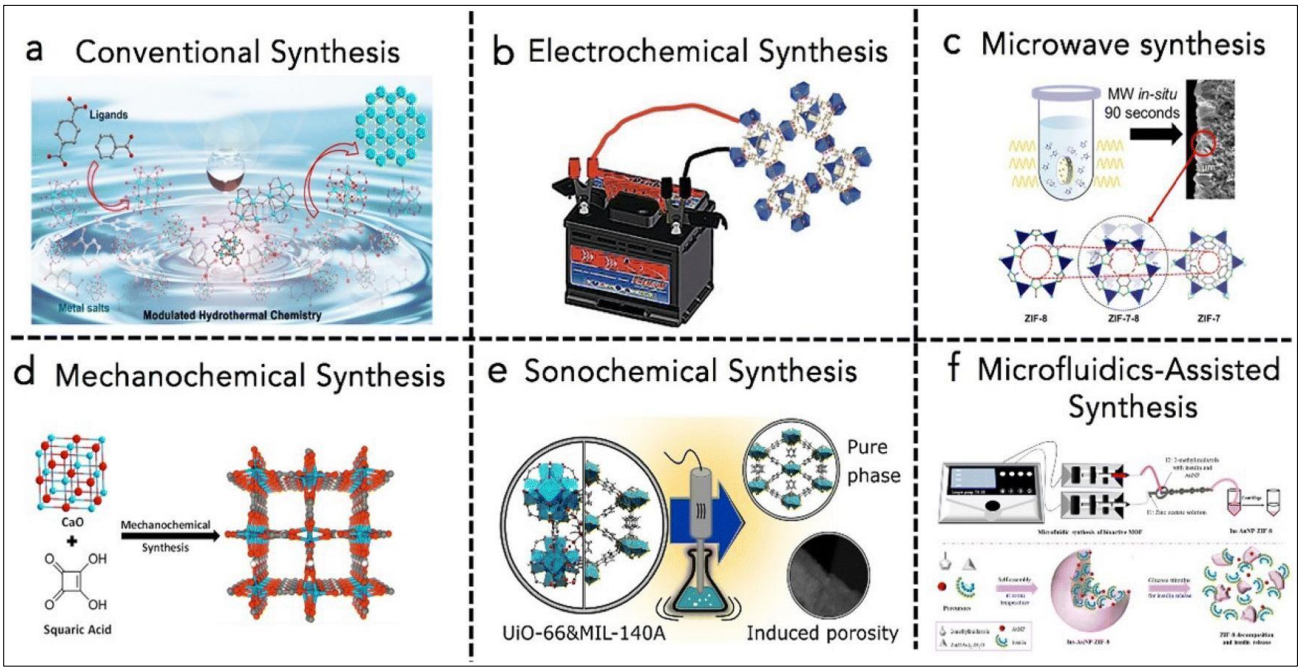

Figure 4: Low-Impact Routes for Sustainable Nanomaterial Fabrication. Lu *et al.,* (2024)

Figure 4 compares conventional hydrothermal processing with microwave-assisted, mechanochemical, sonochemical, electrochemical, and microfluidic fabrication routes. It highlights how alternative energy inputs, reduced solvent consumption, shorter reaction times, and controlled nucleation can support more efficient nanomaterial production.

3.3. Sustainability, Scalability, and Life-Cycle Considerations

Sustainability in multifunctional nanomaterial development cannot be established solely by demonstrating high catalytic activity, adsorption capacity, sensing sensitivity, or electrochemical performance. A complete evaluation must consider the

origin of raw materials, energy and solvent requirements, production yield, worker exposure, material recovery, operational lifetime, and end-of-life fate. Figure 5 illustrates this systems perspective by comparing a conventional cradle-to-grave pathway with circular scenarios in which gold is recovered from nanoparticle waste and returned to production. Such closed-loop strategies replace the linear sequence of synthesis, use, and disposal with recovery, recycling, and repeated utilization (Kang *et al.,* 2024; Khosravi *et al.,* 2024).

Renewable precursors are increasingly being investigated as alternatives to fossil-derived polymers, mined carbon sources, and chemically intensive reducing or stabilizing agents. Cellulose, lignin, chitin, proteins, polysaccharides, plant extracts, and other renewable biomolecules can function as structural building blocks, carbon precursors, reducing agents, capping agents, or surface modifiers. Nanocellulose and lignin nanoparticles are especially attractive because they can be obtained from forestry residues, agricultural waste, and industrial biorefinery side streams while providing tunable surface chemistry, low density, and compatibility with composite fabrication (Österberg *et al.,* 2023).

The use of renewable feedstocks does not automatically guarantee low environmental impact. Biomass cultivation may require land, water, fertilizers, harvesting, transportation, and pretreatment, while conversion into nanomaterials can involve intensive grinding, hydrolysis, solvent extraction, purification, and drying. Feedstock seasonality and chemical variability can also affect particle size, surface functionality, and batch reproducibility. Renewable materials should therefore be selected according to regional availability, competing uses, processing intensity, and their capacity to deliver consistent functional performance rather than simply their biological origin (Österberg *et al.,* 2023; Khosravi *et al.,* 2024).

Waste-derived feedstocks offer additional opportunities to connect nanomaterial production with circular resource management. Agricultural residues, food-processing waste, spent biomass, waste plastics, industrial lignin, sewage-derived materials, and discarded electronic components can be transformed into porous carbons, carbon dots, metal-containing catalysts, adsorbents, and functional composites. This approach can reduce virgin-resource demand and divert waste from disposal, but its sustainability depends on contamination levels, collection requirements, pretreatment, conversion efficiency, and the value of recovered products. Waste valorization is most beneficial when the selected waste stream is abundant, locally available, chemically suitable, and convertible through a limited number of processing stages (Österberg *et al.,* 2023; Modi *et al.,* 2025). A recent scaled-up study of lignin-derived carbon nanoparticles illustrates the importance of integrating waste-derived feedstocks with process-level environmental assessment. Modi et al. (2025) evaluated a continuous, single-step furnace aerosol process for producing porous carbon nanoparticles from lignin and compared it with conventional batch pyrolysis routes through life-cycle assessment. The work is significant because it moves beyond the common laboratory assumption that waste-derived carbon is intrinsically sustainable and instead examines how reactor design, energy demand, residence time, and production scale influence the environmental profile of the final material (Modi *et al.,* 2025).

Energy consumption is frequently one of the dominant environmental hotspots in nanomaterial synthesis. High-temperature calcination, prolonged hydrothermal treatment, inert-gas operation, centrifugation, freeze-drying, solvent evaporation, and repeated washing can consume more energy than the primary chemical reaction. Laboratory equipment may also operate far below its rated capacity, resulting in high energy use per gram of product. Consequently, comparisons among synthesis methods should report energy consumption relative to a defined functional unit, such as one gram of material, one square metre of coated surface, or a specified level of catalytic or storage performance (Patiño-Ruiz *et al.,* 2021; Pilling *et al.,* 2023).

The electricity source must also be considered because an identical synthesis route can produce different greenhouse-gas burdens under different regional energy systems. Reduced reaction time does not necessarily indicate lower energy demand if high-power equipment is used inefficiently. More reliable sustainability assessment requires measurement of actual electricity and thermal-energy consumption, together with evaluation of heat recovery, reactor loading, production yield, and downstream processing. Energy-efficient continuous processing, renewable electricity, process integration, and recovery of waste heat may substantially improve industrial performance when incorporated during early process design (Pilling *et al.,* 2023; Modi *et al.,* 2025).

Solvent selection represents another critical consideration because solvents often dominate the mass input, occupational risk, emissions, and waste-treatment requirements of chemical manufacturing. Replacing volatile organic solvents with water, ethanol, bio-based solvents, ionic liquids, or deep eutectic solvents may reduce some hazards, but a solvent should not be described as green on the basis of low volatility alone. Feedstock origin, toxicity, biodegradability, flammability, recyclability, energy-intensive purification, and life-cycle production burdens must be evaluated together. Some alternative solvents require multistep synthesis or difficult recovery and may transfer environmental burdens to upstream stages (Hessel *et al.,* 2022).

Solvent recovery is therefore often more important than solvent substitution. Closed-loop distillation, membrane separation, phase separation, and direct solvent reuse can reduce both environmental impacts and operating costs. However, recovery systems consume energy and may require additional chemicals, making recovery efficiency and solvent degradation central variables. Industrially credible studies should report solvent-to-product ratios, recovery percentages, purity after recycling, losses per cycle, and changes in nanomaterial quality when recycled solvents are employed (Hessel *et al.,* 2022; Pilling *et al.,* 2023).

Material recovery and recyclability are especially important for nanomaterials containing gold, platinum-group metals, cobalt, nickel, indium, or other scarce and energy-intensive elements. Figure 5 shows that the recovery of gold from nanowaste can return material to nanoparticle synthesis and reduce dependence on pristine gold precursors. In the life-cycle study by Kang et al. (2024), more than 80.4% of the assessed environmental impacts originated from gold nanoparticle synthesis. Reuse reduced the requirement for virgin Au^{3+} despite the additional chemical and electrical inputs associated with recovery, while recovery efficiency was identified as a dominant factor controlling environmental benefit (Kang *et al.,* 2024). Recyclability must be distinguished from theoretical recoverability. A material may contain valuable components but remain difficult to separate from polymers, membranes, electrodes, contaminated water, or complex device assemblies. Effective circular design should therefore incorporate magnetic separation, reversible binding, modular device construction, selective dissolution, regenerable surfaces, and chemically compatible components from the beginning of material development. Repeated recycling must also be tested because particle aggregation, surface oxidation, ligand loss, pore blockage, and compositional changes can reduce performance over successive cycles (Kang *et al.,* 2024; Kim *et al.,* 2024).

Life-cycle assessment provides a systematic method for quantifying environmental burdens across raw-material extraction, synthesis, transportation, use, recovery, and disposal. Its main stages include defining the goal and system boundary, compiling a life-cycle inventory, calculating potential environmental impacts, and interpreting results. Selection of the functional unit is particularly important for nanomaterials because comparison by mass alone may favor materials with poor performance or short lifetimes. Functional units based on contaminant removal, stored energy, catalytic conversion, sensing cycles, or service life can provide more meaningful comparisons among competing technologies (Kang *et al.,* 2024; Patiño-Ruiz *et al.,* 2021).

Patiño-Ruiz et al. (2021) compared plant-mediated and conventional coprecipitation routes for producing iron oxide nanoparticles through a cradle-to-gate assessment. The green route produced lower normalized impacts across the evaluated categories, but the analysis also revealed that ethanol and electricity were major contributors. This result demonstrates why the use of plant extracts cannot, by itself, establish environmental superiority. Purification, heating, solvent consumption, and electricity generation may determine the final environmental profile more strongly than the identity of the reducing agent (Patiño-Ruiz *et al.,* 2021). Industrial-scale production introduces additional challenges involving mixing, heat transfer, pressure control, precursor delivery, product separation, quality assurance, and occupational exposure. Conditions optimized in millilitre-scale experiments may not generate the same nucleation and growth kinetics in larger reactors. Scale-up can alter particle size distributions, defect densities, surface chemistry, and porosity, thereby reducing functional performance. Pilling et al. (2023) proposed that nanomaterial development should jointly consider performance, scalability, environmental effects, and cost rather than optimizing laboratory performance first and addressing manufacturing only afterward (Pilling *et al.,* 2023).

Continuous-flow, aerosol, microreactor, and roll-to-roll manufacturing can improve reproducibility and facilitate industrial production by controlling residence time, mixing, heat transfer, and product collection. Grimaldi et al. (2020) used anticipatory life-cycle assessment to compare continuous-flow and batch production of gold nanoparticles, illustrating the value of evaluating emerging manufacturing routes before commercial infrastructure becomes fixed. However, industrial viability also requires high yield, low off-specification production, reagent recycling, safe handling, and stable material performance across large production volumes (Grimaldi *et al.,* 2020; Pilling *et al.,* 2023). Sustainable industrialization must finally address exposure and end-of-life transformation. Nanomaterials may be released during powder handling, composite machining, product use, recycling, incineration, or landfill disposal, and their properties can change through oxidation, dissolution, aggregation, or interaction with natural organic matter. Life-cycle planning should therefore combine environmental assessment with occupational safety, toxicity evaluation, exposure control, and material-specific disposal strategies. The most credible pathway toward sustainable multifunctional nanomaterials is a circular system that integrates renewable or recovered feedstocks, efficient manufacturing, low-toxicity solvents, long service life, practical regeneration, and validated recovery at the end of use (Kim *et al.,* 2024; Kang *et al.,* 2024).

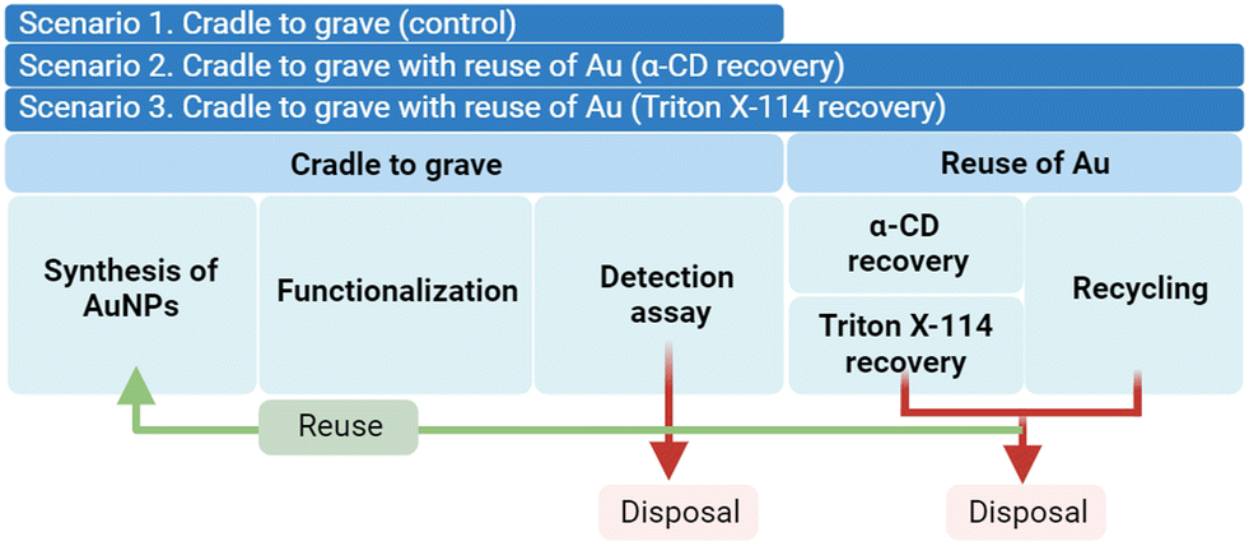

Figure 5: Life-Cycle and Circularity Pathways for Sustainable Nanomaterial Production, Recovery, and Reuse. (Kang *et al.*, 2024)

Figure 5 illustrates the transition from a linear nanomaterial system based on synthesis, use, and disposal to a closed-loop model incorporating nanowaste recovery, recycling, and repeated reuse. It highlights how life-cycle assessment can identify environmental hotspots associated with raw-material consumption, chemical inputs, energy use, recovery efficiency, and end-of-life management.

4. Surface and Interface Engineering of Multifunctional Nanomaterials

4.1. Surface Functionalization, Doping, and Defect Engineering

Surface and interface engineering provides a direct means of controlling the behavior of multifunctional nanomaterials without completely changing their underlying crystal structure or bulk composition. Because a large proportion of atoms in nanoscale materials are located at surfaces, edges, pores, and grain boundaries, their performance is strongly governed by local coordination, surface charge, functional groups, defects, and interactions with surrounding molecules. Chemical functionalization, heteroatom doping, vacancy creation, pore engineering, and ligand modification can therefore regulate dispersibility, adsorption, electron transfer, ion transport, optical response, catalytic activity, and chemical selectivity. These strategies are particularly important for materials intended to perform several functions, such as energy storage, photocatalysis, pollutant removal, and chemical sensing (Bhattacharjee & Prasad, 2023; Mitchell *et al.,* 2021).

Chemical functionalization involves attaching organic or inorganic groups to a nanomaterial surface through covalent bonding, coordination, electrostatic interactions, hydrogen bonding, or π interactions. Functional groups such as hydroxyl, carboxyl, amine, thiol, sulfonate, phosphate, and polymeric chains can modify hydrophilicity, surface charge, colloidal stability, molecular affinity, and compatibility with other phases. For environmental applications, carboxyl, amine, and sulfur-containing groups can increase binding toward metal ions and polar contaminants. In electrochemical systems, conductive polymers or redox-active molecules may improve charge transfer, while hydrophilic groups facilitate electrolyte penetration and ion accessibility (Bhattacharjee & Prasad, 2023; Sun *et al.,* 2025).

Covalent functionalization provides strong and durable surface attachment but may disrupt the electronic structure of carbon-based or two-dimensional materials. For example, converting sp^2-hybridized carbon atoms into sp^3 centers can introduce scattering sites and reduce conductivity. Noncovalent functionalization generally preserves the intrinsic lattice more effectively and allows reversible modification, but the attached species may desorb under changes in temperature, pH, ionic strength, or solvent composition. Selection between covalent and noncovalent approaches must therefore reflect the required balance among functional stability, electrical performance, processability, and regeneration (Sun *et al.,* 2025).

Ligand modification represents a specialized form of surface functionalization that is especially important for metallic nanoparticles, quantum dots, and colloidal nanocrystals. Ligands coordinate exposed surface atoms, suppress aggregation, regulate crystal growth, and determine interactions between the nanocrystal and its environment. A ligand typically contains a surface-binding group and an outward-facing molecular segment that controls solubility, steric stabilization, self-assembly, and chemical recognition. Ligand identity and surface coverage can also influence the electronic states of the nanocrystal, meaning that ligands should be regarded as functional components of

the complete material rather than passive coatings (Giansante, 2020; Bhattacharjee & Prasad, 2023).

Long-chain organic ligands can produce stable colloidal dispersions but may create insulating barriers that restrict electron transport and block surface-active sites. Ligand exchange with shorter organic molecules, inorganic ions, or electronically conductive species can reduce interparticle separation and improve device conductivity. In catalysis, partial ligand removal may increase reactant access, although complete removal can trigger nanoparticle aggregation or expose unstable surfaces. Ligands may also enhance catalytic activity by modifying adsorption through steric, electronic, and solubility effects, showing that their influence cannot be described simply as beneficial or detrimental (Lu *et al.,* 2021).

Heteroatom doping introduces foreign atoms into a host lattice or carbon network to alter charge distribution, bonding configuration, carrier concentration, and chemical reactivity. In carbon materials, nitrogen, boron, sulfur, phosphorus, oxygen, and fluorine are frequently used as dopants. Nitrogen can form pyridinic, pyrrolic, graphitic, and oxidized configurations, each producing a different electronic environment. Boron is electron deficient relative to carbon, while nitrogen is more electronegative; their incorporation can therefore generate polarized sites that promote adsorption and electron transfer. Sulfur and phosphorus can introduce larger atomic distortions and influence spin or charge density around neighboring atoms (Wang *et al.,* 2020).

Single-element doping can adjust one dominant property, whereas dual or multiple heteroatom doping may generate cooperative effects through complementary electronic perturbations. In porous carbons, doping can improve wettability, create pseudocapacitive sites, increase affinity toward gases or pollutants, and modify catalytic reaction pathways. However, functional performance depends on dopant configuration, concentration, accessibility, and thermal stability rather than elemental content alone. A high nominal dopant concentration may provide limited benefit when the atoms are buried within inaccessible regions or occupy chemically inactive configurations (Wang *et al.,* 2020).

Doping also applies to metal oxides, semiconductors, quantum dots, and layered materials. Substitutional dopants can introduce charge carriers, modify bandgap energy, extend optical absorption, and alter magnetic or catalytic properties. Aliovalent doping may require charge compensation through vacancies or changes in oxidation state, linking doping directly with defect formation. Excessive dopant loading can produce secondary phases, lattice instability, carrier trapping, or recombination centers. Reliable interpretation therefore requires identifying dopant location and oxidation state through methods such as X-ray photoelectron spectroscopy, electron energy-loss spectroscopy, X-ray absorption spectroscopy, and atomically resolved microscopy.

Defect engineering deliberately creates or regulates vacancies, interstitial atoms, dislocations, grain boundaries, antisite defects, edges, and under-coordinated surface sites. These imperfections disrupt periodic atomic arrangements and produce localized electronic states that may change adsorption energies, band structure, carrier mobility, and redox activity. Vacancies are particularly important because removing an atom exposes unsaturated neighboring sites and may redistribute charge across the surrounding lattice. Oxygen vacancies in metal oxides can promote molecular activation and visible-light absorption, while sulfur or selenium vacancies can activate otherwise less reactive basal planes of transition-metal dichalcogenides (Muhammad *et al.,* 2024; Su *et al.,* 2023).

Vacancies can be introduced through thermal treatment, reduction, plasma processing, chemical etching, irradiation, mechanical strain, or controlled nonstoichiometric synthesis. The effects depend on vacancy type, concentration, spatial distribution, and stability under operating conditions. Moderate concentrations may improve charge separation and create active sites, whereas excessive vacancies can weaken the lattice, increase nonradiative recombination, accelerate corrosion, or interrupt conductive pathways. Defect engineering should therefore aim for controlled and characterizable defect populations rather than maximizing disorder indiscriminately (Muhammad *et al.,* 2024).

Defects and dopants often function cooperatively. A heteroatom may distort the local lattice and promote nearby vacancy formation, while a vacancy may stabilize a dopant or isolated metal atom. This interaction can generate active centers with electronic structures unavailable in pristine materials. Defect sites can also anchor metal nanoparticles or single atoms, limiting migration and aggregation during catalytic operation. In multifunctional systems, the same defect may improve catalytic reactivity and chemical sensing by increasing analyte adsorption, although it may reduce long-term stability during repeated electrochemical cycling (Mitchell *et al.,* 2021; Muhammad *et al.,* 2024).

Pore engineering regulates pore size, pore volume, connectivity, geometry, and surface chemistry to control molecular transport and active-site accessibility. Micropores provide strong adsorption and high internal surface area, mesopores support movement of solvated ions and larger molecules, and macropores facilitate fluid transport and reduce diffusion resistance. Hierarchical architectures combining multiple pore scales are therefore advantageous for catalysts, adsorbents, electrodes, membranes, and sensors. Their

performance depends not only on total surface area but on whether the pore network is accessible to the intended ions, reactants, or contaminants (Bennett *et al.,* 2021; Wang *et al.,* 2020).

Porosity can be introduced through hard templates, soft templates, activation, selective etching, phase separation, self-assembly, gas evolution, or conversion of porous precursors. In MOFs and COFs, pore size and internal chemical functionality can be adjusted through building-block selection and post-synthetic modification. In carbon materials, chemical or physical activation creates high surface area, but aggressive activation may weaken the framework, reduce conductivity, and generate nonuniform pores. Effective pore engineering must therefore balance surface area, mass transport, volumetric density, electrical continuity, and mechanical stability (Bennett *et al.,* 2021; Wang *et al.,* 2020).

Control of surface-active sites is the ultimate objective connecting functionalization, doping, defects, pores, and ligands. An active site is defined not merely by elemental composition but by its coordination environment, electronic state, accessibility, and interaction with neighboring atoms or functional groups. Surface engineering can increase the number of active sites, alter their intrinsic activity, or create microenvironments that selectively concentrate reactants. Site-selective modification may also generate Janus or patchy nanoparticles whose different surface regions perform distinct functions, including molecular capture, catalysis, assembly, or signal generation (Mitchell *et al.,* 2021; Lu *et al.,* 2021).

4.2. Hetero structures and Interfacial Charge-Transfer Mechanisms

Hetero structure engineering involves integrating two or more materials with dissimilar electronic structures to create interfaces that regulate charge generation, migration, separation, and consumption. In multifunctional nanomaterials, these interfaces may form between two semiconductors, a metal and semiconductor, a metal and oxide support, or a conductive carbon phase and a catalytic component. Their effectiveness depends on band alignment, work-function differences, Fermi-level positions, interfacial bonding, contact area, defects, and structural compatibility. Properly designed heterointerfaces can suppress electron-hole recombination, accelerate electron transport, stabilize active phases, and preserve charge carriers with sufficient energy for surface reduction and oxidation reactions (Sayed *et al.,* 2025; Leybo *et al.,* 2024).

Semiconductor heterojunctions are commonly classified according to the semiconducting nature and band alignment of their components. Figure 6 presents four possible S-scheme combinations involving n-type and p-type oxidation and reduction photocatalysts: n-n, p-p, p-n, and n-p heterojunctions. In each configuration, the oxidation photocatalyst possesses relatively lower Fermi, conduction-band, and valence-band energy levels, whereas the reduction photocatalyst generally possesses a higher Fermi level and a more negative conduction-band position. These energetic differences provide the initial driving force for interfacial electron redistribution after physical contact (Sayed *et al.,* 2025).

Before contact, the constituent semiconductors retain their independent Fermi levels and band structures. Once intimate contact is established, electrons migrate from the reduction photocatalyst with the higher Fermi level toward the oxidation photocatalyst with the lower Fermi level until electronic equilibrium is reached. This redistribution creates an electron-depleted region on the reduction photocatalyst and an electron-accumulated region on the oxidation photocatalyst. The resulting positively and negatively charged interfacial layers generate band bending and a built-in interfacial electric field directed from the reduction photocatalyst toward the oxidation photocatalyst, as represented in Figure 6 (Sayed *et al.,* 2025).

Under light irradiation, both semiconductors absorb photons with sufficient energy to excite electrons from their valence bands to their conduction bands. The built-in electric field, band bending, and Coulombic attraction then favor the recombination of relatively low-energy electrons in the conduction band of the oxidation photocatalyst with relatively weakly oxidizing holes in the valence band of the reduction photocatalyst. Consequently, highly reducing electrons remain in the conduction band of the reduction photocatalyst, while strongly oxidizing holes remain in the valence band of the oxidation photocatalyst. This pathway combines spatial charge separation with preservation of strong redox potentials, allowing the remaining carriers to drive hydrogen evolution, carbon dioxide reduction, oxygen activation, or pollutant oxidation (Sayed *et al.,* 2025).

This mechanism differs from conventional type-II heterojunctions. In an idealized type-II system, photogenerated electrons migrate to the semiconductor with the lower conduction-band energy, while holes accumulate in the material with the higher valence-band energy. Although this arrangement can spatially separate carriers, it may retain electrons and holes with weaker reduction and oxidation abilities. S-scheme systems instead eliminate carriers with relatively limited redox power and preserve those located at more energetically favorable band positions. Nevertheless, the assignment of an S-scheme mechanism should be supported experimentally because apparent improvements in photocatalytic performance do not, by themselves, establish the direction of charge migration (Sayed *et al.,* 2025).

The quality of the semiconductor interface strongly influences whether thermodynamically

favorable charge transfer occurs at a useful rate. Inadequate contact area, lattice mismatch, interfacial contamination, insulating residues, and poorly connected particles can create transport barriers that promote charge trapping and recombination. Conversely, coherent interfaces, chemical bonds, and closely integrated nanostructures can decrease charge-transfer distance and increase electronic coupling. Deng *et al.,* (2024) constructed electrospun In_2O_3/Nb_2O_5 S-scheme nanofibers with intimate interphase contact and observed interfacial electron transfer occurring in less than 10 ps through femtosecond transient-absorption spectroscopy. The system retained electrons in the Nb_2O_5 conduction band and holes in the In_2O_3 valence band with prolonged carrier lifetimes, improving carbon dioxide photoreduction (Deng *et al.,* 2024).

Interfacial chemical bonds can provide defined pathways for electron migration and stabilize contact between dissimilar phases. Wang *et al.,* (2021) reported a sulfur-vacancy-rich $ZnIn_2S_4/MoSe_2$ heterostructure in which interfacial Mo-S bonding, sulfur vacancies, and an internal electric field cooperatively regulated Z-scheme charge transfer. Surface photovoltage spectroscopy, electron-paramagnetic-resonance measurements, and density-functional-theory calculations supported the proposed interfacial mechanism. The study demonstrates that heterostructure formation is most effective when electronic coupling, defect chemistry, and built-in fields are engineered together rather than treated as independent design variables (Wang *et al.,* 2021).

Internal electric fields may also be established within a single phase or between crystallographic domains and then coupled with a semiconductor heterojunction. Wan *et al.,* (2024) combined zinc-blende/wurtzite superlattice interfaces within $Mn_{0.5}Cd_{0.5}S$ nanorods with S-scheme interfaces formed between the nanorods and $MnWO_4$ nanoparticles. The superlattice interfaces promoted bulk charge separation, while the surface heterojunction accelerated interfacial separation and transfer. The combined architecture achieved a hydrogen-evolution rate of 54.4 mmol g^{-1} h^{-1} and an apparent quantum efficiency of 63.1% at 420 nm, illustrating how multiple interfacial fields can operate across different length scales (Wan *et al.,* 2024).

Metal-semiconductor interfaces introduce additional charge-transfer mechanisms. When a metal contacts a semiconductor, differences in their work functions can cause electron migration and produce a Schottky barrier, band bending, and a space-charge region. Metals may act as electron sinks, cocatalytic reaction sites, or plasmonic light absorbers, thereby reducing bulk recombination and facilitating surface reactions. However, an excessively high interfacial barrier or abundant trap states may slow electron extraction and increase energy loss. Wang, Xue, and Chen (2019) showed that semiconductor-cocatalyst electron transfer is sensitive to the electronic structure of the contact and that unfavorable potential barriers can kinetically limit photocatalytic reactions despite apparently suitable thermodynamics (Wang *et al.,* 2019).

Metal-support interactions extend beyond simple electron trapping. Oxide supports can donate or withdraw charge, stabilize isolated atoms and clusters, modify metal adsorption energies, participate directly in reactions, or partially encapsulate metal nanoparticles under reducing conditions. These interactions may evolve dynamically during thermal treatment or catalytic operation as the metal oxidation state, support defects, adsorbates, and local atomic structure change. Therefore, the catalyst-support interface should be regarded as an active reaction region rather than an inert boundary between a metal particle and carrier material (Leybo *et al.,* 2024).

Direct evidence for such charge redistribution was provided by Zachman *et al.,* (2022) using Au nanoparticles supported on $SrTiO_3$. Four-dimensional scanning transmission electron microscopy simultaneously mapped atomic structure and nanoscale charge distribution, showing electron transfer from the support to pristine Au nanoparticles. Oxygen-based post-synthesis treatment reversed the transfer direction and altered catalytic behavior. Charge redistribution was concentrated near particle perimeters, supporting the view that metal-support boundaries can generate chemically distinct active sites whose electronic properties differ from those of the particle interior or unmodified support (Zachman *et al.,* 2022).

Carbon-metal interfaces are especially important in electrocatalysis, energy storage, and sensing because conductive carbons can disperse metals, form continuous electron pathways, and modify the electronic states of supported particles. Graphene, carbon nanotubes, porous carbons, and heteroatom-doped carbon frameworks contain defects and functional groups capable of anchoring metals through coordination or covalent interactions. Nitrogen, sulfur, phosphorus, and oxygen dopants change the local charge density and work function of carbon, thereby regulating the direction and magnitude of interfacial electron transfer.

Yan *et al.,* (2019) demonstrated that charge transfer between platinum and sulfur-doped carbon depended on metal size. Electrons moved from isolated Pt atoms toward the sulfur-doped support because of strong Pt-S interactions, whereas sulfur-doped carbon donated electrons to Pt when the metal was enlarged to clusters of approximately 1.5 nm. The electron-enriched Pt clusters exhibited stronger hydrogen-evolution performance than the electron-deficient single atoms. This finding confirms that carbon-metal charge transfer depends not only on support chemistry but also on metal nuclearity, coordination, and interfacial geometry (Yan *et al.,* 2019).

The construction of an effective heterointerface must therefore balance thermodynamic driving forces with kinetic accessibility. Appropriate band positions may predict a favorable charge-transfer direction, but actual performance also depends on carrier diffusion length, interface resistance, trap-state density, contact intimacy, surface reaction rate, and competition between productive transfer and recombination. A large interfacial area can improve carrier extraction, although excessive boundaries may create defects that act as recombination centers. Similarly, strong chemical bonding can accelerate transfer but may introduce structural distortion or modify band positions in ways that reduce redox capability.

Accurate identification of interfacial mechanisms requires complementary characterization rather than reliance on a single band diagram. Ultraviolet photoelectron spectroscopy and Kelvin-probe measurements can estimate work functions and Fermi levels, while Mott-Schottky analysis assists in identifying semiconductor type and flat-band potential. X-ray photoelectron and absorption spectroscopies reveal chemical bonding and charge redistribution, whereas surface photovoltage, time-resolved photoluminescence, transient-absorption spectroscopy, and electrochemical impedance measurements evaluate carrier separation and transfer kinetics. Electron-paramagnetic-resonance spin trapping can identify reactive species, and density-functional-theory calculations can relate interfacial structure to charge-density differences and adsorption energetics (Sayed *et al.,* 2025; Zachman *et al.,* 2022).

Heterostructure performance ultimately depends on the coordinated design of electronic alignment, physical contact, chemical bonding, interfacial electric fields, and accessible reaction sites. Semiconductor heterojunctions can preserve energetic electrons and holes, metal-semiconductor contacts can facilitate carrier extraction, metal-support interactions can regulate adsorption and stability, and carbon-metal interfaces can provide conductive and electronically tunable networks. These mechanisms establish interfaces as central functional elements in nanomaterials designed for photocatalysis, electrocatalysis, energy storage, environmental remediation, and chemical sensing.

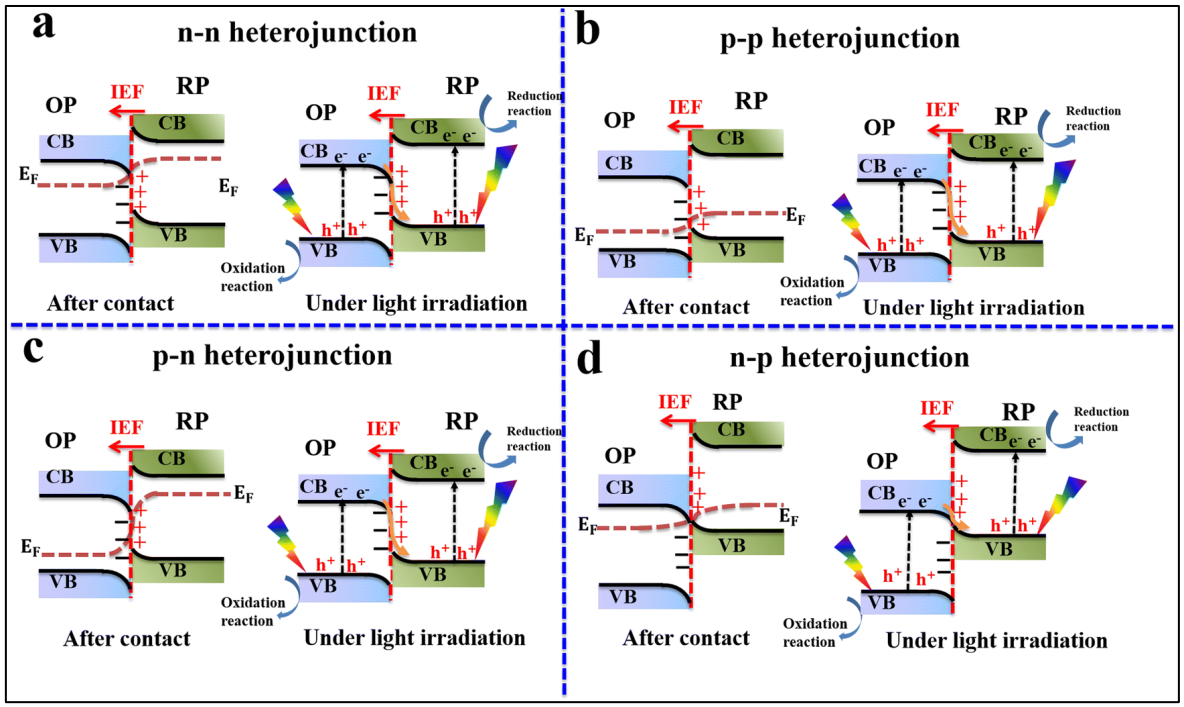

Figure 6: Interfacial Electric Fields and Charge-Transfer Pathways in Multifunctional Hetero structures. Sayed *et al.,* (2025)

Figure 6 illustrates how contact between oxidation and reduction photocatalysts causes Fermi-level equilibration, interfacial charge redistribution, band bending, and formation of a built-in electric field. Under illumination, this field promotes directional charge migration, selective carrier recombination, and spatial separation of strongly reducing electrons and strongly oxidizing holes.

4.3. Advanced Characterization of Surfaces and Interfaces

Accurate characterization of multifunctional nanomaterials requires the integration of microscopic, structural, spectroscopic, surface, porosity, and electrochemical measurements. No single technique can independently reveal particle morphology, atomic arrangement, chemical state, pore accessibility, interfacial charge transfer, and dynamic behavior under

operating conditions. Figure 7 distinguishes material-focused methods, which examine crystallinity and electronic or geometric structure, from intermediate-focused methods that identify adsorbed species and reaction products. This distinction is important because the material characterized after synthesis may differ substantially from the active structure formed during catalysis, electrochemical cycling, sensing, or pollutant treatment. A multimodal strategy is therefore essential for establishing reliable structure-property-performance relationships (Mourdikoudis *et al.,* 2018; Prajapati *et al.,* 2025).

Electron microscopy provides direct information about particle size, morphology, aggregation, interfaces, and spatial distribution. Scanning electron microscopy is particularly useful for examining surface texture, particle organization, coatings, porous networks, and fracture morphology across relatively large areas. Transmission electron microscopy offers higher spatial resolution and can reveal particle dimensions, internal structures, core-shell architectures, grain boundaries, lattice fringes, and interfacial contact between nanocomposite components. High-resolution TEM and scanning TEM can approach atomic-scale imaging, while selected-area electron diffraction assists in phase and crystallographic analysis. When combined with energy-dispersive X-ray spectroscopy or electron energy-loss spectroscopy, electron microscopy can map elemental distribution, oxidation-state variation, and chemical heterogeneity at interfaces (Mourdikoudis *et al.,* 2018; Wang *et al.,* 2023).

Electron microscopy data must nevertheless be interpreted carefully. Drying, vacuum exposure, sample-section preparation, and electron irradiation may modify soft materials, hydrated interfaces, surface ligands, oxidation states, or defect populations. Images acquired from a small field of view may also fail to represent the overall particle population. Reliable analysis should therefore include images from several locations, statistically meaningful size distributions, and complementary measurements such as XRD, gas adsorption, or bulk elemental analysis. Liquid-cell and environmental electron microscopy can reduce the gap between static imaging and operating conditions, but electron-beam-induced radiolysis, heating, reduction, or structural damage may still create transformations that are mistaken for intrinsic material behavior (Mourdikoudis *et al.,* 2018; Prajapati *et al.,* 2025).

Atomic force microscopy provides three-dimensional surface topography by monitoring the interaction between a sharp probe and the sample. It can determine particle height, surface roughness, layer thickness, pore openings, aggregation, and local mechanical properties under ambient or liquid conditions. Force-spectroscopy modes provide information about adhesion, elasticity, deformation, and tip-surface interactions, while conductive AFM and Kelvin probe force microscopy map local conductivity, surface potential, work-function differences, and charge heterogeneity. These capabilities are valuable for analyzing semiconductor junctions, catalytic interfaces, electrode coatings, membranes, and two-dimensional materials whose electronic behavior varies across grains or defects (Mourdikoudis *et al.,* 2018; Checa *et al.,* 2023).

Advanced Kelvin probe force microscopy can extend AFM from static imaging to dynamic charge analysis. Checa et al. (2023) introduced a sparse-scanning approach that enabled sub-second mapping of nanoscale charge behavior and visualization of oxygen-vacancy motion in polycrystalline TiO_2. Such developments are highly relevant to multifunctional materials because ionic migration, surface charging, and local potential gradients can regulate photocatalysis, sensing, electrochemical storage, and interface degradation. However, AFM measurements remain sensitive to tip geometry, feedback conditions, humidity, sample preparation, and tip-induced deformation. Apparent lateral dimensions may be broadened by tip convolution, making complementary electron microscopy or independent dimensional measurements necessary (Checa *et al.,* 2023).

X-ray diffraction identifies crystalline phases, lattice symmetry, unit-cell parameters, preferred orientation, and structural transformations. Peak positions indicate interplanar spacings and phase composition, whereas peak widths can provide approximate information about coherent crystallite dimensions and microstrain when appropriate models are applied. XRD is particularly important for detecting phase purity, dopant-induced lattice changes, interlayer expansion, thermal transformations, and conversion between crystalline states. Its principal limitation is its reliance on long-range order. Amorphous phases, ultrasmall clusters, surface layers, and low-concentration interfacial species may produce broad or weak signals that are difficult to distinguish from the background (Mourdikoudis *et al.,* 2018; Prajapati *et al.,* 2025).

In situ and operando XRD can monitor phase evolution while a material is exposed to temperature, gas, electrolyte, illumination, or applied potential. These measurements can reveal reversible lattice expansion, phase conversion, crystallization, structural degradation, and metal-oxide reduction during operation. X-ray absorption spectroscopy provides complementary element-specific information when long-range crystallinity is absent. X-ray absorption near-edge structure is sensitive to electronic state and coordination geometry, while extended X-ray absorption fine structure probes the local coordination number, bond distance, and disorder surrounding selected atoms. Combining diffraction with absorption spectroscopy therefore links bulk phase evolution with local electronic

and atomic changes (Wang *et al.,* 2023; Prajapati *et al.,* 2025).

X-ray photoelectron spectroscopy is one of the most widely applied methods for characterizing the outer surface of nanomaterials. It provides elemental composition, chemical-state information, relative oxidation states, and evidence of bonding interactions within the upper few nanometres of a material. Changes in binding energy can indicate charge redistribution, ligand coordination, heteroatom doping, vacancy-associated states, and interfacial interaction between composite components. Depth profiling and angle-resolved measurements can investigate compositional gradients, while ultraviolet photoelectron spectroscopy can provide information about valence-band structure and work function. These data are central to constructing band alignments and interpreting charge-transfer mechanisms in heterostructures (Isaacs *et al.,* 2021).

XPS is also susceptible to overinterpretation. Binding energies may be influenced by charging, calibration procedures, final-state effects, sample conductivity, peak overlap, and differential surface contamination. Curve fitting should therefore use physically justified peak shapes, constrained chemical assignments, appropriate backgrounds, and reference materials where possible. Apparent oxidation-state changes inferred from small binding-energy shifts should be supported by complementary spectroscopy, elemental analysis, or theoretical calculations. Isaacs et al. (2021) emphasized that combining XPS with ultraviolet photoelectron spectroscopy, Auger spectroscopy, ion scattering, and electron-energy-loss measurements can provide a more complete understanding than routine peak fitting alone (Isaacs *et al.,* 2021).

Raman spectroscopy probes vibrational modes and is sensitive to crystal symmetry, molecular bonding, structural disorder, strain, phase composition, and surface adsorbates. In carbon materials, the D, G, and related bands provide information about disorder, graphitic domains, and defect-related scattering. In metal oxides and layered materials, changes in peak position, width, and intensity may indicate phase transformation, layer number, strain, doping, or vacancy formation. Raman mapping can visualize chemical heterogeneity across a surface, while surface-enhanced Raman spectroscopy strengthens signals from species located near plasmonic metals, enabling the detection of low-coverage intermediates at catalytic interfaces (Prajapati *et al.,* 2025; Wang *et al.,* 2023).

Fourier-transform infrared spectroscopy complements Raman analysis by detecting vibrations associated with functional groups, surface ligands, adsorbed molecules, and chemical intermediates. Hydroxyl, carbonyl, carboxyl, amine, phosphate, and metal-oxygen-related bands can confirm functionalization and provide evidence of contaminant binding or ligand exchange. Attenuated-total-reflectance FTIR is useful for films and interfaces, while diffuse-reflectance and surface-enhanced infrared methods can examine powders, catalysts, and adsorbates under controlled atmospheres. Raman and FTIR follow different selection rules, so vibrations weak in one method may be prominent in the other. Their combined use produces a more complete description of surface bonding and reaction pathways (Wang *et al.,* 2023; Prajapati *et al.,* 2025).

Brunauer-Emmett-Teller analysis uses gas-adsorption isotherms to estimate specific surface area, while related models provide pore volume and pore-size distribution. Nitrogen adsorption at 77 K is widely used for porous carbons, oxides, MOFs, COFs, catalysts, and adsorbents. The shape and hysteresis of the adsorption-desorption isotherm can reveal aspects of microporosity, mesoporosity, capillary condensation, and structural flexibility. However, BET area should not be treated as an absolute descriptor of functional performance because inaccessible pores, pore connectivity, surface chemistry, adsorbate size, and activation conditions influence the measured result and practical accessibility (Nazari *et al.,* 2024).

The reproducibility of BET calculations is a significant concern. A multi-laboratory study using the same adsorption datasets showed substantial variation in calculated areas when analysts selected different pressure ranges and fitting points. Transparent reporting should therefore include the complete isotherm, degassing conditions, adsorptive gas, temperature, selected relative-pressure range, fitting criteria, and pore-analysis model. Algorithms such as BET surface identification can improve consistency, but careful inspection of the raw adsorption isotherm remains essential, particularly for flexible and microporous materials (Osterrieth *et al.,* 2022; Nazari *et al.,* 2024).

Electrochemical characterization connects material structure with charge-storage, catalytic, and sensing behavior. Cyclic voltammetry identifies redox processes, reversibility, capacitive contributions, and potential-dependent surface transformations. Galvanostatic charge-discharge measurements provide capacity, capacitance, rate capability, coulombic efficiency, and cycling stability. Linear-sweep voltammetry and Tafel analysis are used to evaluate electrocatalytic activity and kinetic response, while chronopotentiometry and chronoamperometry assess stability at controlled current or potential. These measurements require careful normalization by catalyst mass, geometric area, electrochemically active area, or accessible surface area because different normalizations can produce substantially different performance interpretations (Prajapati *et al.,* 2025).

Electrochemical impedance spectroscopy applies a small alternating perturbation across a range of

frequencies to separate processes occurring at different characteristic timescales. Equivalent-circuit or physics-based analysis can provide estimates of electrolyte resistance, interfacial charge-transfer resistance, capacitance, diffusion behavior, and contact limitations. However, several circuits may fit the same data, so circuit selection must be physically justified and accompanied by uncertainty analysis and residual evaluation. System stability, linearity, frequency range, perturbation amplitude, and reproducibility should be confirmed before mechanistic conclusions are drawn (Wang *et al.,* 2021).

In situ characterization measures a material while it experiences a controlled stimulus, whereas operando characterization simultaneously monitors structural or chemical changes and functional performance under working conditions. Figure 7 highlights this integration by linking the applied stimulus, catalyst response, spectroscopic signal, reactant conversion, and product formation. Operando methods are particularly important because catalysts and electrodes may reconstruct, change oxidation state, accumulate adsorbates, dissolve, or form new active phases during use. Ex situ measurements performed before and after operation may miss short-lived intermediates and reversible transformations that control activity (Prajapati *et al.,* 2025; Wang *et al.,* 2023).

Operando experiments introduce their own limitations. Optical windows, thin electrolyte layers, restricted cell geometries, and probe-access requirements may create mass-transport, pressure, temperature, or current-density conditions that differ from conventional performance tests. Gas bubbles may block the active surface or interfere with X-ray and optical measurements, while intense X-rays, lasers, and electron beams can modify the sample. The catalytic or electrochemical performance of the operando cell must therefore be measured and compared with a benchmark reactor. Reactor dimensions, flow conditions, electrode loading, transport characteristics, and probe exposure should also be reported to establish whether the observed behavior is representative of practical operation (Prajapati *et al.,* 2025).

A reliable characterization framework consequently requires deliberate cross-validation. Electron microscopy and AFM resolve morphology and local properties; XRD identifies crystalline phases; XPS determines surface composition and chemical states; Raman and FTIR reveal bonding, defects, and intermediates; BET analysis quantifies accessible porosity; and electrochemical methods evaluate transport and functional kinetics. In situ and operando measurements then establish how these characteristics evolve during operation. Combining these methods with theoretical calculations and statistically representative sampling reduces mechanistic overreach and supports defensible relationships between surface structure, interface chemistry, and multifunctional performance (Mourdikoudis *et al.,* 2018; Prajapati *et al.,* 2025).

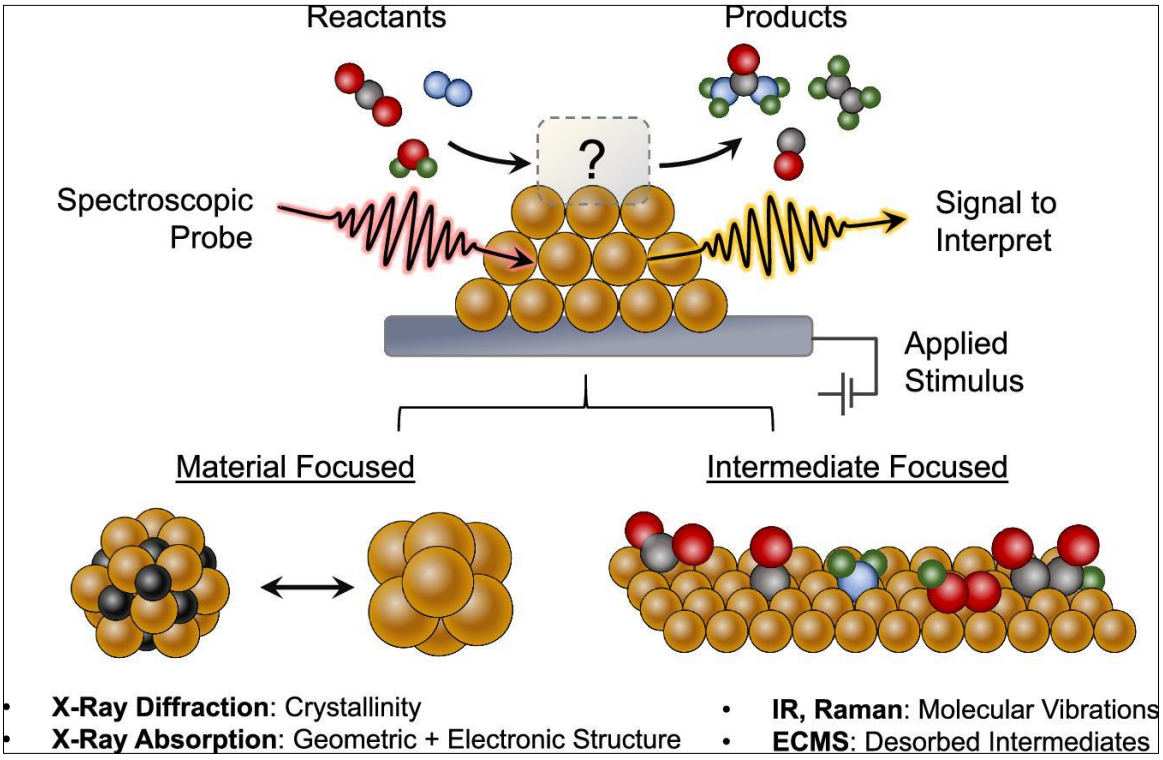

Figure 7: Multimodal Characterization of Nanomaterial Surfaces and Interfaces: From Atomic Structure to Operando Function. Prajapati et al. (2025)

Figure 7 illustrates how complementary microscopic, structural, spectroscopic, surface, porosity, and electrochemical techniques reveal nanomaterial morphology, crystallinity, chemical states, functional groups, surface area, charge-transfer behavior, and reaction intermediates. It also highlights the transition from static ex situ measurements to in situ and operando analysis of surfaces and interfaces under realistic working conditions.

5. Catalytic and Photocatalytic Applications

5.1. Fundamentals of Nanomaterial-Based Catalysis

Nanomaterial-based catalysis exploits the high surface-to-volume ratio, tunable electronic structure, structural diversity, and abundance of low-coordination atoms in nanoscale solids to accelerate chemical reactions. Heterogeneous nanocatalysts commonly include supported metal nanoparticles, isolated metal atoms, metal oxides, porous frameworks, carbon-based materials, and multicomponent nanocomposites. Unlike homogeneous catalysts, these materials generally exist in a phase different from the gaseous or liquid reactants, allowing relatively straightforward separation and reuse. Their performance is determined not only by chemical composition but also by particle size, morphology, exposed facets, crystallinity, defect concentration, porosity, and interactions between the active phase and its support. Nanoscale engineering can therefore regulate catalytic activity, selectivity, stability, and resistance to deactivation with a level of structural control that is difficult to achieve in conventional bulk materials (Liu & Corma, 2018; Mitchell *et al.,* 2021).

Catalytic active sites are localized atomic configurations where reactant adsorption, bond activation, intermediate transformation, and product formation occur. In metal nanoparticles, these sites may consist of surface terraces, steps, edges, corners, kinks, or interfacial atoms possessing coordination numbers and electronic structures distinct from those of bulk atoms. In metal oxides, active sites may include oxygen vacancies, coordinatively unsaturated metal centres, lattice oxygen, Brønsted or Lewis acid sites, and adjacent acid-base pairs. Carbon-based catalysts may derive activity from heteroatom dopants, edge defects, vacancies, or metal-nitrogen coordination environments. Consequently, the total surface area of a nanomaterial does not necessarily represent its catalytically useful area because only a fraction of exposed atoms may possess the appropriate geometry and electronic configuration for a specific reaction (Li *et al.,* 2020; Vogt & Weckhuysen, 2022).

Single-atom catalysts represent the limiting case of nanoscale dispersion, in which individual metal atoms are anchored to a support through coordination with oxygen, nitrogen, sulfur, carbon, or lattice atoms. Such systems can theoretically maximize metal utilization and create relatively uniform coordination environments. However, the surrounding support, neighbouring defects, ligands, solvent molecules, and adsorbates frequently participate in the reaction. The active site should therefore be considered a cooperative and dynamic ensemble rather than a permanently fixed isolated atom. Under working conditions, single atoms may migrate, change coordination or oxidation state, or aggregate into clusters and nanoparticles. Conversely, nanoparticles may redisperse into smaller species. These transformations can alter activity and selectivity, meaning that ex situ characterization alone may not identify the actual working catalyst (Liu *et al.,* 2019; Sarma *et al.,* 2023).

Adsorption initiates most heterogeneous catalytic cycles by bringing reactant molecules into contact with active surface sites. Physisorption is dominated by relatively weak electrostatic and van der Waals interactions, whereas chemisorption involves stronger orbital interactions, charge transfer, or chemical-bond formation between the adsorbate and catalyst. Adsorption energy influences surface coverage, molecular orientation, bond polarization, and the likelihood that an adsorbed species will proceed toward a transition state. Defects, dopants, lattice strain, exposed crystal planes, interfacial electric fields, and metal-support charge transfer can modify adsorption strength and thereby change the preferred reaction pathway. Competitive adsorption is also important because solvents, reaction products, impurities, and intermediates may occupy the same active sites as the desired reactants.

Optimal catalytic behaviour generally follows the Sabatier principle, according to which reactants and intermediates should bind strongly enough to become activated but not so strongly that they permanently block the surface. If adsorption is too weak, reactant coverage and activation remain insufficient. If adsorption is excessively strong, intermediates accumulate, products cannot desorb efficiently, and active sites become poisoned. This relationship frequently produces volcano-type activity trends when reaction rates are plotted against adsorption-energy descriptors. Particle-size regulation, alloy formation, surface functionalization, heteroatom doping, defect engineering, and support selection provide practical strategies for positioning adsorption energies closer to their catalytic optimum (Mitchell *et al.,* 2021; van Deelen *et al.,* 2019).

Desorption completes the catalytic turnover by releasing products and regenerating vacant sites. A surface may activate reactants effectively yet exhibit low turnover if products or stable intermediates remain strongly adsorbed. Desorption kinetics are affected by temperature, pressure, solvent, surface coverage, and lateral interactions among adsorbates. In porous nanocatalysts, molecular transport introduces additional complexity. Micropores can enhance adsorption and molecular discrimination, but narrow channels may restrict diffusion and limit accessibility to internal active sites. Hierarchical architectures containing

interconnected micro-, meso-, and macropores can alleviate these constraints by combining high surface area with shorter diffusion pathways. Distinguishing intrinsic surface kinetics from external mass transfer and intraparticle diffusion is therefore essential when comparing nanocatalyst performance.

Catalysts accelerate reactions by providing alternative elementary pathways with lower activation free-energy barriers, while leaving the overall thermodynamic equilibrium unchanged. Barrier reduction may result from bond weakening during adsorption, stabilization of charged or radical intermediates, transition-state stabilization, proton-coupled electron transfer, dissociative adsorption, or cooperative activation at neighbouring sites. Catalytic kinetics are commonly evaluated using conversion, reaction rate, turnover frequency, reaction order, apparent activation energy, and selectivity. Turnover frequency normalizes activity to the estimated number of active sites, although uncertainty in identifying and counting these sites can complicate comparisons among structurally different nanomaterials. Apparent activation energies can also contain contributions from adsorption equilibria, surface coverage, diffusion, and structural changes, and therefore should not automatically be interpreted as the barrier of a single elementary step.

Microkinetic modelling links individual adsorption, desorption, surface-reaction, and diffusion steps to experimentally observed rates and product distributions. Density functional theory can calculate adsorption energies and transition-state barriers, while microkinetic analysis determines which elementary steps exert the greatest kinetic control under specific temperatures, pressures, potentials, and surface coverages. The classical concept of a single rate-determining step is often insufficient for complex nanocatalytic networks because control may be distributed across several elementary processes and may shift as operating conditions change. Reliable mechanistic conclusions therefore require integration of kinetic measurements with isotopic labelling, transient analysis, theoretical calculations, and in situ or operando spectroscopy (Kiani & Wachs, 2024b; Sarma *et al.,* 2023).

Selectivity arises from competition among parallel and sequential reaction pathways. Nanomaterial structure can favour a desired pathway by selectively stabilizing particular adsorbates or transition states, regulating reactant orientation, controlling the availability of neighbouring sites, or restricting molecular transport. Isolated metal atoms may suppress side reactions that require large metallic ensembles, whereas specific transformations require pairs or larger groups of adjacent atoms. Bimetallic nanoparticles can combine complementary functions, such as dissociating hydrogen on one component and activating an oxygenated substrate on another. Similarly, interfaces between metals and reducible oxides can redistribute charge, create new adsorption configurations, supply lattice oxygen, and stabilize selected oxidation states. Nevertheless, excessively strong metal-support interactions may partially encapsulate nanoparticles and reduce the number of accessible sites, illustrating the need to balance electronic promotion with physical accessibility (van Deelen *et al.,* 2019).

Several mechanistic models describe heterogeneous catalytic reactions. In the Langmuir-Hinshelwood mechanism, two reactants adsorb before reacting on the surface. The reaction rate therefore depends on adsorption equilibria, surface coverage, and the availability of neighbouring sites. Recent analysis has emphasized that the widely used concept of identical "pair sites" can be misleading for structurally heterogeneous catalysts, particularly when two chemically distinct sites cooperate in a bimolecular reaction (Kiani & Wachs, 2024a). In the Eley-Rideal mechanism, a gas-phase or solution-phase reactant reacts directly with an adsorbed species. However, distinguishing a true direct-collision pathway from rapid weak adsorption or precursor-mediated behaviour requires rigorous kinetic and spectroscopic evidence (Kiani & Wachs, 2024b).

Metal-oxide catalysts may operate through a Mars-van Krevelen mechanism, in which lattice oxygen reacts directly with an adsorbed substrate, creating an oxygen vacancy that is subsequently replenished by molecular oxygen. Catalytic activity in this mechanism depends on oxide reducibility, vacancy-formation energy, oxygen mobility, and reoxidation kinetics. Other systems may follow acid-base, redox, bifunctional, or interfacial pathways in which different components catalyse successive elementary steps. Multiple mechanisms can coexist, and their relative importance may change with surface coverage, temperature, pressure, solvent composition, or applied electrochemical potential.

Overall, effective nanocatalyst design requires simultaneous optimization of active-site density, intrinsic reactivity, adsorption strength, product desorption, molecular transport, selectivity, and structural stability. A large surface area alone cannot guarantee superior performance because catalytic behaviour ultimately depends on the identity and dynamics of accessible working sites. Establishing quantitative relationships among atomic structure, adsorption energetics, activation barriers, reaction kinetics, and product selectivity provides the mechanistic foundation for applying multifunctional nanomaterials in chemical synthesis, environmental remediation, electrocatalysis, and photocatalytic energy conversion.

5.2. **Photocatalytic Energy Conversion**

Photocatalytic energy conversion uses semiconductor materials to transform solar radiation into

chemical energy stored in hydrogen, oxygen-linked redox products, carbon monoxide, methane, methanol, and other renewable fuels. As illustrated in Figure 8, the process begins when incident photons with energies equal to or greater than the semiconductor bandgap excite electrons from the valence band to the conduction band, leaving positively charged holes in the valence band. The photogenerated electrons and holes subsequently migrate toward surface reaction sites, where they drive reduction and oxidation reactions, respectively. Their useful participation competes directly with bulk and surface recombination, which dissipates absorbed photon energy as heat or luminescence without producing chemical products (Gong *et al.,* 2022; Takata *et al.,* 2020).

The energetic positions of the conduction-band minimum and valence-band maximum determine whether a semiconductor can support a desired redox transformation. For overall water splitting, the conduction band must provide electrons with sufficient reducing power for proton reduction, whereas the valence band must contain holes capable of oxidizing water. Thermodynamically, water splitting requires at least 1.23 eV under standard conditions, but practical photocatalysts require a larger energy input because of overpotentials, charge-transfer resistance, recombination, and surface kinetic barriers. A narrow bandgap improves visible-light absorption, but excessive narrowing may weaken the reduction or oxidation ability of the charge carriers. Photocatalyst design must therefore balance broad solar absorption with sufficiently strong band-edge redox potentials (Takata *et al.,* 2020; Lin *et al.,* 2024).

Photocatalytic hydrogen generation occurs when conduction-band electrons reduce protons or water molecules to molecular hydrogen. The corresponding holes must be consumed through water oxidation or, in laboratory studies, through oxidation of sacrificial electron donors. Although sacrificial systems are useful for evaluating hydrogen-evolution activity, they do not constitute complete solar-fuel cycles because the consumed reagent supplies part of the chemical energy. True overall water splitting couples hydrogen evolution with oxygen evolution in the stoichiometric ratio of 2:1. Cocatalysts such as Pt, Rh/Cr_2O_3, Ni-based species, and other reduction-active nanoparticles can trap electrons, reduce hydrogen-evolution overpotentials, and suppress competing back reactions when selectively deposited on appropriate surface sites.

A major advance was achieved using Al-doped $SrTiO_3$ modified with spatially separated Rh/Cr_2O_3 and CoOOH cocatalysts for hydrogen and oxygen evolution, respectively. This facet-selective arrangement exploited anisotropic charge migration and achieved an external quantum efficiency of up to 96% between 350 and 360 nm, corresponding to an internal quantum efficiency approaching unity. The result demonstrated that nearly all absorbed photons can theoretically be used for overall water splitting when charge separation and surface redox reactions are carefully coordinated. However, the photocatalyst remained primarily responsive to ultraviolet light, emphasizing that high quantum efficiency alone does not ensure high solar-to-hydrogen efficiency unless a substantial portion of the visible solar spectrum is also utilized (Takata *et al.,* 2020).

Oxygen evolution is generally more kinetically demanding than hydrogen evolution because it involves the accumulation of four holes, multiple proton-transfer events, formation of oxygen-oxygen bonds, and release of O_2. Slow oxygen-evolution kinetics can cause holes to accumulate, increasing charge recombination and promoting photocorrosion. Oxidation cocatalysts accelerate interfacial hole transfer and reduce the energetic barrier for water oxidation. Spatially separating oxidation and reduction sites also limits the reverse reaction between H_2 and O_2. In Z-scheme systems, two light-absorbing photocatalysts are connected through a soluble redox mediator or solid electron conductor, allowing low-energy electrons and holes to recombine while preserving strongly reducing electrons on the hydrogen-evolution photocatalyst and strongly oxidizing holes on the oxygen-evolution photocatalyst.

Recent Z-scheme designs illustrate the importance of complementary band structures. Lin et al. (2024) combined $Sm_2Ti_2O_5S_2$ as a visible-light-responsive hydrogen-evolution photocatalyst with $BiVO_4$ as the oxygen-evolution component and reduced graphene oxide as the solid electron mediator. After surface modification to improve charge separation and redox kinetics, the system maintained overall water splitting for more than 100 h and achieved a solar-to-hydrogen efficiency of 0.22%. This configuration shows how tandem light absorbers can extend spectral utilization while retaining the strong redox potentials required for both half-reactions (Lin *et al.,* 2024).

Bandgap engineering is central to improving photocatalytic energy conversion. Elemental doping can introduce donor or acceptor states, shift band edges, or extend absorption into the visible region, although uncontrolled defect states may become recombination centres. Solid-solution formation, anion substitution, vacancy engineering, strain regulation, quantum confinement, and construction of semiconductor heterojunctions provide additional control over optical absorption and carrier transport. In organic photocatalysts, the electronic structure can be adjusted through molecular building blocks, conjugation length, framework polarity, and donor-acceptor architecture. For example, donor-acceptor engineering in covalent organic framework nanosheets reduced exciton-binding limitations, prolonged charge-carrier lifetimes, and produced an apparent quantum efficiency of 82.6% at 450 nm for sacrificial hydrogen evolution with a Pt cocatalyst (Li *et al.,* 2022).

Light harvesting depends not only on the intrinsic bandgap but also on optical path length, absorption coefficient, particle morphology, surface scattering, and exciton behaviour. Nanostructured arrays, hollow particles, porous frameworks, two-dimensional sheets, plasmonic metals, and photonic architectures can increase light capture by promoting multiple scattering or concentrating electromagnetic fields near reactive interfaces. Plasmonic nanoparticles may generate energetic carriers or local electromagnetic enhancement under visible irradiation, whereas conjugated polymers and frameworks allow molecular-level tuning of absorption. Nevertheless, expanded light absorption is beneficial only when the additional excited carriers can be separated, transported, and transferred to reactants before recombination. This requirement explains why Figure 8 identifies limited absorption and charge recombination as interconnected rather than independent barriers.

Photocatalytic carbon dioxide reduction extends solar-fuel chemistry beyond hydrogen by converting CO_2 into CO, formate, methanol, methane, and multicarbon products. The reaction is more complex than proton reduction because CO_2 is chemically stable, poorly adsorbed by many semiconductor surfaces, and capable of following multiple proton-coupled electron-transfer pathways. Two-electron pathways generally yield CO or formate, whereas methanol and methane require six and eight electrons, respectively. Multicarbon products require additional carbon-carbon coupling steps. Product selectivity therefore depends on CO_2 adsorption geometry, intermediate binding strength, proton availability, local charge density, active-site structure, and suppression of the competing hydrogen-evolution reaction.

Figure 8 accordingly identifies CO_2 adsorption and activation, reaction-mechanism determination, and C_1/C_2 selectivity as major limitations. Porous photocatalysts can improve CO_2 enrichment near active centres, while metal sites, vacancies, ionic liquids, and surface functional groups can stabilize activated intermediates such as *COOH and *CO. Wang et al. (2024) integrated CO_2-enriching ionic liquids into visible-light-responsive PCN-250 metal-organic frameworks. The optimized host-guest material achieved CO-formation rates of 313.34 μmol g^{-1} h^{-1} under pure CO_2 and 153.42 μmol g^{-1} h^{-1} under 15% CO_2, with approximately 100% selectivity. The ionic liquid enriched CO_2 and cooperated with Co^{2+} sites to reduce the free-energy barrier of the rate-controlling conversion step (Wang *et al.,* 2024).

Selectivity under realistic gas compositions is especially challenging because oxygen can capture photogenerated electrons more readily than CO_2. Ma et al. (2022) addressed this limitation by coating hollow TiO_2 with microporous Pd-porphyrin-based polymers, producing an environment that enhanced CO_2 uptake and regulated charge transfer under aerobic conditions. Such designs show that solar-fuel performance depends on simultaneous control of photon absorption, reactant concentration, carrier migration, catalytic-site chemistry, and competitive reactions. Photocatalytic systems must also be carefully evaluated through carbon-free controls and isotopic labelling because carbon-containing catalysts, solvents, and residual synthesis reagents can otherwise produce misleading carbon products (Ma *et al.,* 2022).

Photothermal-photocatalytic coupling provides another route for using a broader fraction of the solar spectrum. Ren et al. (2024) developed oxygen-vacancy-rich CeO_2 containing isolated Ni sites for concentrated solar conversion of CO_2 and water vapour to methane. The material achieved a solar-to-chemical efficiency of 1.14%, a methane yield of 192.75 μmol cm^{-2} h^{-1}, and approximately 100% selectivity. Oxygen vacancies supplied active sites, while isolated Ni centres promoted charge capture and water activation. This example demonstrates that coordinated use of photogenerated carriers and solar-derived heat can lower apparent activation barriers and improve full-spectrum solar utilization, although concentrated-light operation introduces additional requirements for thermal stability and reactor engineering (Ren *et al.,* 2024).

Practical implementation ultimately requires photocatalysts that combine efficient visible-light absorption, rapid charge separation, selective surface chemistry, photochemical stability, scalable fabrication, and safe product separation. A 100 m^2 $SrTiO_3$:Al panel-reactor array demonstrated outdoor overall water splitting and autonomous hydrogen separation with a maximum solar-to-hydrogen efficiency of 0.76%, confirming the technical feasibility of large-area particulate photocatalysis while also revealing remaining efficiency and economic limitations (Nishiyama *et al.,* 2021). Thus, Figure 8 accurately presents photocatalytic energy conversion as an integrated sequence in which bandgap engineering, light harvesting, carrier dynamics, reactant activation, selectivity, and durability must be optimized together rather than individually.

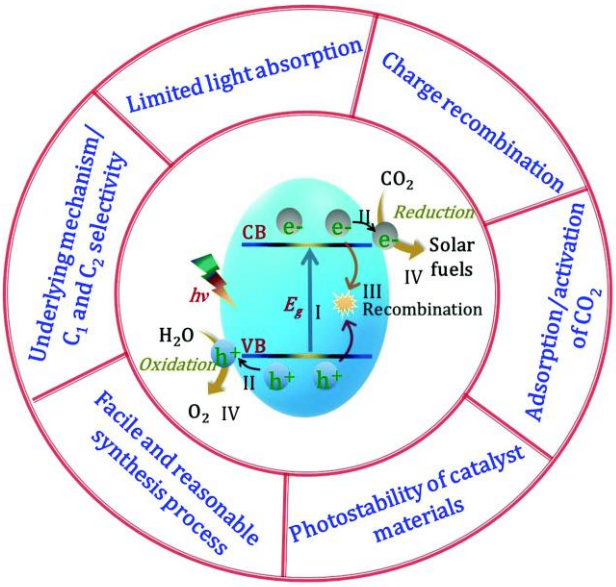

Figure 8: Band-Engineered Charge Dynamics for Photocatalytic Solar-Fuel Generation. Gong *et al.*, (2022)

The figure illustrates photon absorption across a semiconductor bandgap, electron-hole generation, charge migration and recombination, and the subsequent surface redox reactions that reduce CO_2 into solar fuels while oxidizing water to O_2. It highlights how light harvesting, band alignment, carrier separation, surface activation, selectivity, and photostability collectively determine photocatalytic energy-conversion efficiency.

5.3. **Photocatalytic Environmental Remediation**

Photocatalytic environmental remediation applies light-responsive semiconductor nanomaterials to transform persistent contaminants into less harmful compounds through advanced oxidation and reduction processes. Unlike adsorption, which mainly transfers pollutants from water to a solid phase, photocatalysis can chemically decompose contaminant molecules and potentially mineralize them into carbon dioxide, water, and inorganic ions. The process has been widely investigated for synthetic dyes, pharmaceuticals, pesticides, antibiotics, endocrine-disrupting compounds, and other contaminants of emerging concern that are incompletely removed by conventional wastewater treatment systems (Koe *et al.,* 2020; Gopinath *et al.,* 2020).

As illustrated in Figure 9, irradiation of a semiconductor with photons of energy equal to or greater than its bandgap promotes electrons from the valence band to the conduction band and leaves positively charged holes in the valence band. Conduction-band electrons can reduce dissolved oxygen to superoxide radicals, while valence-band holes may directly oxidize adsorbed pollutants or react with water and hydroxide ions to produce hydroxyl radicals. Further electron- and proton-transfer reactions can generate hydrogen peroxide, hydroperoxyl radicals, and singlet oxygen. These reactive oxygen species differ in lifetime, selectivity, diffusion distance, and oxidation potential, so the dominant degradation mechanism depends on the photocatalyst composition, band positions, pollutant structure, water chemistry, and irradiation conditions (Rangarajan *et al.,* 2022; Lu *et al.,* 2022).

Hydroxyl radicals are highly reactive and can attack aromatic rings, unsaturated bonds, and electron-rich functional groups with limited selectivity. Superoxide radicals generally exhibit weaker oxidation ability but can participate in reduction, oxygen activation, and subsequent formation of hydrogen peroxide and hydroxyl radicals. Singlet oxygen may contribute through more selective reactions with electron-rich organic structures, while photogenerated holes can initiate direct oxidation at the catalyst surface. Radical-scavenging experiments, electron paramagnetic resonance spectroscopy, isotope labelling, and probe-molecule analysis are therefore necessary to identify the dominant active species. Scavenger tests alone should be interpreted cautiously because scavengers can also alter adsorption, surface charge, and light absorption (Rangarajan *et al.,* 2022; Subhiksha *et al.,* 2022).

Figure 9 demonstrates that biochar-supported semiconductors can combine contaminant adsorption with photocatalytic degradation. The porous carbon matrix concentrates organic molecules near reactive sites through electrostatic attraction, hydrogen bonding, hydrophobic interactions, and π-π interactions. Its conjugated domains may also function as electron acceptors or transport pathways, thereby limiting electron-hole recombination. Persistent free radicals, quinone-like groups, dissolved organic matter, and oxygen-containing functionalities in biochar may additionally participate in oxygen activation and reactive-species formation. The illustrated systems include representative pathways for contaminants such

as diethyl phthalate, bisphenol A, tetracycline, and rhodamine B, highlighting that pollutant removal results from the combined effects of adsorption, charge separation, interfacial electron transfer, and reactive oxygen species generation (Lu *et al.,* 2022).

Synthetic dyes are frequently used as model pollutants because their degradation can be monitored conveniently through the disappearance of characteristic visible absorption bands. Photocatalytic oxidation can cleave azo bonds, disrupt conjugated chromophores, remove substituent groups, and open aromatic rings. Nevertheless, colour disappearance should not be equated with complete degradation or detoxification. A dye may lose its chromophore while producing colourless aromatic amines, aldehydes, carboxylic acids, or other transformation products that remain environmentally hazardous. Accordingly, dye-removal studies should combine ultraviolet-visible spectroscopy with total organic carbon, chemical oxygen demand, chromatographic analysis, and toxicity evaluation to distinguish decolorization from mineralization (Chen *et al.,* 2020; Khan *et al.,* 2024).

The degradation rate of dyes depends strongly on catalyst loading, solution pH, dye concentration, light intensity, and interactions between charged dyes and the catalyst surface. Cationic and anionic dyes may display very different adsorption and degradation behaviour on the same photocatalyst because the surface charge changes relative to the point of zero charge. Excessive catalyst loading can reduce performance by increasing turbidity, particle aggregation, and light scattering, whereas insufficient loading limits the number of accessible active sites. Dye molecules may also photosensitize a semiconductor by absorbing visible light and transferring electrons into its conduction band, which can produce apparently high degradation rates that do not necessarily represent intrinsic photocatalyst activity (Koe *et al.,* 2020; Khan *et al.,* 2024).

Pharmaceuticals and antibiotics present a more demanding remediation challenge because they occur at relatively low concentrations in complex water matrices and often contain chemically stable aromatic, halogenated, or heterocyclic structures. Compounds such as acetaminophen, ibuprofen, diclofenac, carbamazepine, sulfamethoxazole, ciprofloxacin, tetracycline, and amoxicillin have consequently become important targets for heterogeneous photocatalysis. Metal oxides, graphitic carbon nitride, carbon-based composites, bismuth-containing semiconductors, metal-organic frameworks, and heterojunction photocatalysts have been developed to extend visible-light absorption and improve interfacial charge separation (Srivastava, 2024; Subhiksha *et al.,* 2022).

Antibiotic degradation is environmentally significant because residual antimicrobial activity may promote microbial selection and dissemination of antibiotic-resistance determinants. Photocatalytic treatment must therefore eliminate both the original antibiotic and the biological activity of its transformation products. Oxidative pathways may involve hydroxylation, dealkylation, decarboxylation, defluorination, cleavage of carbon-nitrogen bonds, and opening of heterocyclic rings. Wang et al. (2021), for example, developed an N-doped carbon-coated cobalt-manganese oxide capable of activating peroxymonosulfate under visible light for the treatment of several pharmaceutical compounds, including tetracycline, norfloxacin, carbamazepine, metronidazole, and amoxicillin. The carbon coating improved light utilization, charge separation, mass transfer, and control of metal leaching, demonstrating the value of integrating photocatalysis with photo-Fenton-like oxidation.

Pesticides can be particularly resistant to biological treatment because they are intentionally designed to retain biological activity and environmental stability. Photocatalysis can attack chlorinated aromatic rings, nitro groups, heterocyclic structures, and other persistent moieties, but degradation efficiency varies with pesticide adsorption and molecular structure. Tariq *et al.,* (2023) reported 92.3% degradation of the neonicotinoid pesticide imidacloprid using an Ag_2O/CuO composite under optimized ultraviolet irradiation. Superoxide radicals, electrons, and hydroxyl radicals contributed to the process, and gas chromatography-mass spectrometry was used to investigate degradation. However, activity declined from 92.3% in the first cycle to 78% and 63.41% in the second and third cycles, respectively, illustrating that catalyst reusability cannot be inferred solely from high initial removal efficiency.

Mineralization is generally achieved through sequential oxidation rather than a single-step reaction. The parent contaminant is first converted into hydroxylated, dealkylated, dehalogenated, or ring-opened intermediates, which are subsequently oxidized into short-chain carboxylic acids and finally into carbon dioxide, water, nitrate, ammonium, sulfate, phosphate, or halide ions. Some intermediates can be more toxic, mobile, or biologically active than the original compound. Consequently, high-performance studies should report total organic carbon removal, identify intermediates using liquid chromatography-mass spectrometry or gas chromatography-mass spectrometry, propose plausible reaction pathways, and assess residual ecotoxicity or antimicrobial activity (Gopinath *et al.,* 2020; Srivastava, 2024).

Catalyst recovery is a central requirement for practical implementation because dispersed nanoparticles are difficult to separate from treated water and may introduce secondary contamination. Magnetic photocatalysts containing Fe_3O_4, ferrites, or other magnetic phases can be collected using an external magnetic field. Immobilization on glass, ceramics,

fibres, biochar, membranes, foams, and polymeric supports can also simplify recovery and enable continuous-flow operation. However, immobilization may decrease effective surface area and introduce mass-transfer limitations, while magnetic components may promote charge recombination or metal leaching if interfaces are not carefully engineered (Zheng *et al.,* 2024).

Reusability must be evaluated through repeated cycles accompanied by structural, chemical, and leaching analyses. Declining activity may arise from nanoparticle aggregation, photocorrosion, surface fouling, pore blockage, loss of active components, or accumulation of strongly adsorbed intermediates. Washing, thermal regeneration, chemical oxidation, or solvent treatment may restore activity, but the environmental and energetic costs of regeneration should be included in sustainability assessments. Stable performance over a few cycles under idealized laboratory conditions is insufficient to demonstrate long-term applicability in real wastewater.

Natural organic matter, carbonate, bicarbonate, chloride, sulfate, phosphate, and suspended particles can compete for active sites, absorb incident light, or quench reactive oxygen species. Real effluents also contain mixtures of contaminants that compete for adsorption and oxidation, making degradation slower and less predictable than in single-pollutant laboratory solutions. Future photocatalytic systems should therefore be evaluated at environmentally relevant concentrations under solar irradiation, realistic hydraulic conditions, and complex water chemistry. Overall, Figure 9 emphasizes that effective photocatalytic remediation requires the coordinated optimization of pollutant adsorption, light harvesting, charge separation, reactive-species production, mineralization, catalyst recovery, and long-term reusability.

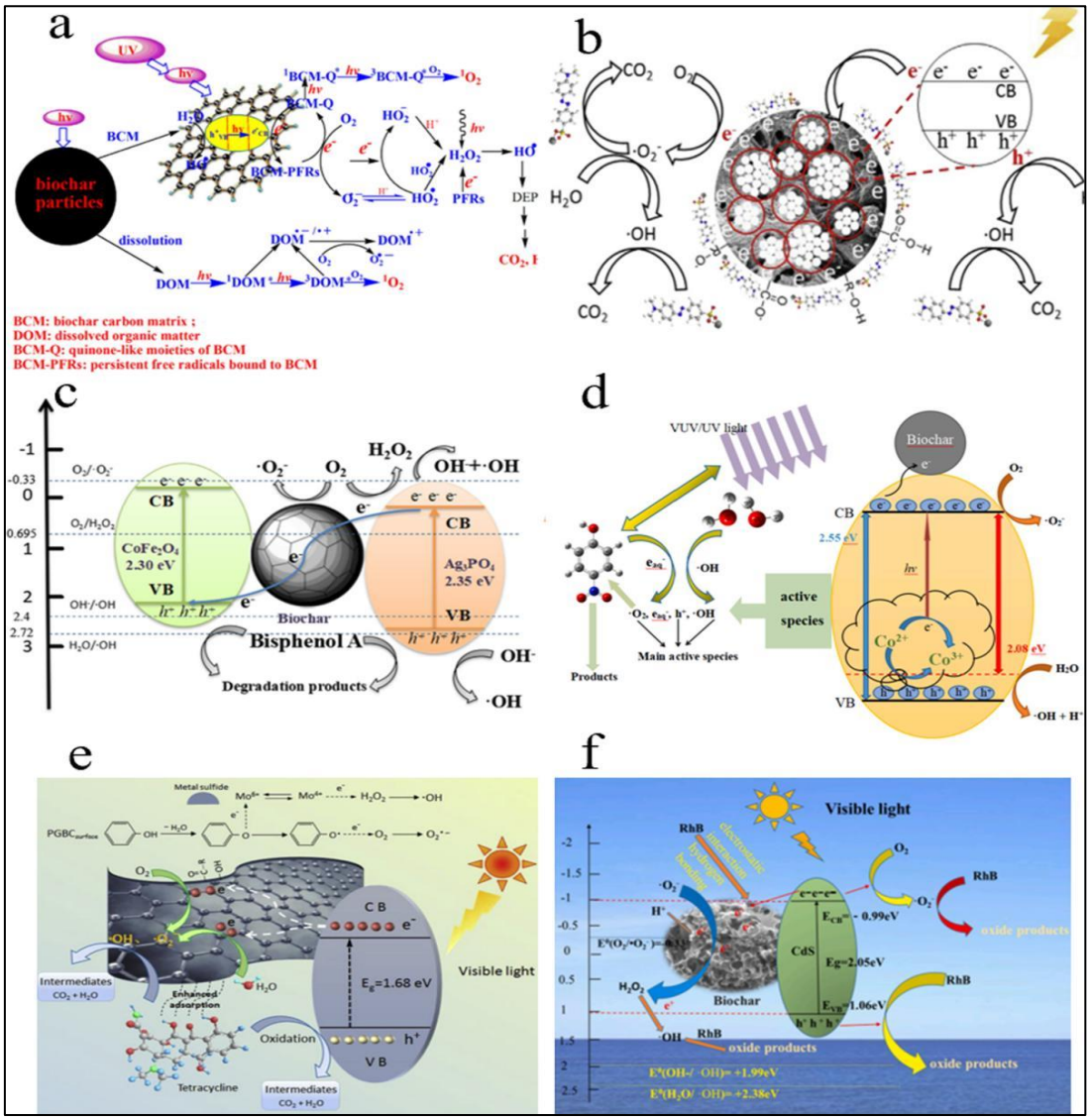

Figure 9: Reactive-Oxygen-Species Pathways for Photocatalytic Degradation and Mineralization of Emerging Pollutants

The figure illustrates how light-induced electron-hole separation in nanomaterial-based photocatalysts generates hydroxyl radicals, superoxide radicals, singlet oxygen, and other oxidative species that transform dyes, antibiotics, pharmaceuticals, and persistent organic contaminants into smaller intermediates and, ideally, CO_2 and H_2O. It also highlights the synergistic roles of pollutant adsorption, interfacial charge transfer, band alignment, and visible-light activation in improving remediation efficiency.

6. Electrochemical Energy-Storage Applications

6.1. Nanomaterials for Rechargeable Batteries

Rechargeable batteries store electrical energy through reversible redox reactions accompanied by ion transport between positive and negative electrodes. The electrochemical performance of these systems is controlled by electrode capacity, operating voltage, ionic and electronic conductivity, interfacial stability, and the reversibility of structural transformations during repeated charge and discharge. Nanostructured materials are particularly valuable because shortened solid-state diffusion distances, enlarged electrode-electrolyte contact areas, tunable pore networks, and abundant active sites can improve ion-transfer kinetics and active-material utilization. Nanoparticles, nanowires, nanosheets, hollow structures, porous carbons, and hybrid nanocomposites can also accommodate mechanical strain and maintain conductive pathways during cycling. However, excessive surface area may accelerate electrolyte decomposition, interphase growth, dissolution, and parasitic reactions, indicating that nanoscale design must balance kinetic enhancement with chemical stability (Manthiram, 2020; Popovic, 2021).

Lithium-ion batteries remain the dominant rechargeable technology because lithium possesses a small ionic radius, low redox potential, and favourable gravimetric capacity. Commercial cathodes are primarily based on layered oxides, spinels, and polyanion compounds, whereas graphite is the conventional anode. Layered $LiCoO_2$ and nickel-manganese-cobalt oxides provide relatively high voltages and capacities, spinel materials offer three-dimensional Li^+ diffusion, and $LiFePO_4$ combines structural stability with long cycle life. Nanoscale particles shorten Li^+ diffusion pathways and can improve high-rate performance, while conductive carbon coatings compensate for the low intrinsic conductivity of many polyanion materials. Nevertheless, very small particles increase interfacial reactivity and reduce electrode tap density, which may lower volumetric energy density despite improved gravimetric kinetics (Manthiram, 2020).

High-capacity lithium-ion anodes based on silicon, tin, transition-metal oxides, and other alloying or conversion materials can store more lithium than graphite. Their practical application is restricted by substantial volume changes, particle fracture, electrical disconnection, and repeated rupture and reformation of the solid-electrolyte interphase. Nanostructured Si particles, porous frameworks, yolk-shell structures, elastic binders, and carbon matrices provide internal void space and mechanical confinement, reducing stress accumulation while maintaining electrical contact. These designs improve capacity retention, but their high surface area can consume additional electrolyte and lithium during interphase formation, producing low initial Coulombic efficiency.

Lithium-ion battery degradation involves interconnected chemical, electrochemical, thermal, and mechanical processes. Growth of the solid-electrolyte interphase consumes cyclable lithium and increases resistance, while electrolyte oxidation at high cathode potentials produces gases and unstable cathode-electrolyte interphases. Nickel-rich layered cathodes can undergo oxygen release, transition-metal dissolution, surface reconstruction, and anisotropic lattice changes that generate intergranular microcracks. Fast charging or low-temperature operation may also cause metallic lithium plating on graphite, increasing capacity loss and internal-short-circuit risk. These mechanisms produce loss of lithium inventory, loss of active material, increased impedance, and eventual power and capacity fade (Edge *et al.,* 2021).

Sodium-ion batteries employ a rocking-chair mechanism similar to lithium-ion batteries but use more abundant sodium resources. Their cathode candidates include layered transition-metal oxides, polyanion compounds, and Prussian blue analogues, while hard carbon is the most widely investigated anode. Layered sodium oxides can deliver favourable capacities but frequently undergo multiple phase transitions and slab gliding as Na^+ ions are extracted and inserted. Polyanion frameworks offer structural robustness and thermal stability, whereas Prussian blue analogues possess open three-dimensional channels that promote sodium transport. Their performance can nevertheless be limited by structural water, vacancy defects, low density, and dissolution of transition-metal species (Abraham, 2020).

Because Na^+ is larger and heavier than Li^+, electrode structures require wider diffusion channels and greater tolerance to strain. Nanostructuring can reduce Na^+ diffusion distances and improve the rate performance of poorly conducting electrode materials, while carbon coating and heteroatom doping enhance electronic conductivity. Hard carbon contains disordered graphene domains, nanopores, defects, and expanded interlayer spacing that enable sodium adsorption, intercalation, and pore filling. However, its high surface area and defect concentration can promote irreversible electrolyte decomposition, resulting in low initial Coulombic efficiency. Cycling degradation in sodium-ion cells additionally arises from unstable interphases, cathode phase transformations, transition-metal migration, particle cracking, and continuous electrolyte consumption.

Potassium-ion batteries are attractive because potassium is abundant and the K^+/K redox couple permits relatively high cell voltages in non-aqueous electrolytes. Unlike sodium, potassium can be reversibly intercalated into graphite, making graphite a potentially practical low-cost anode. Other electrode candidates include hard carbons, layered oxides, Prussian blue analogues, organic materials, metal chalcogenides, and alloying compounds based on antimony, bismuth, tin, and phosphorus. The large K^+ ion, however, generates severe structural strain and slow solid-state transport in compact lattices. Nanoporous carbon architectures, expanded-layer compounds, hollow particles, and flexible carbon-supported composites can facilitate K^+ movement and buffer repeated volume changes (Hosaka *et al.,* 2020).

Potassium-ion battery stability is closely associated with the electrode-electrolyte interface. Potassium is highly reactive, and the resulting solid-electrolyte interphase may be chemically heterogeneous, mechanically unstable, or partially soluble. Alloying and conversion anodes can undergo pronounced expansion, pulverization, and loss of electrical contact, whereas layered cathodes may experience irreversible phase transitions and transition-metal dissolution. Electrolyte additives, concentrated electrolytes, artificial interphases, surface coatings, and nanoscale strain-accommodating structures are therefore required to improve Coulombic efficiency and suppress continuous interfacial degradation (Hosaka *et al.,* 2020; Popovic, 2021).

Aqueous zinc-ion batteries combine a metallic zinc anode with cathodes such as manganese oxides, vanadium oxides, Prussian blue analogues, organic compounds, and layered materials. They offer intrinsic non-flammability, low material cost, and high ionic conductivity. Zn^{2+} storage can proceed through insertion, conversion, coordination, dissolution-deposition, or coupled H^+/Zn^{2+} mechanisms. Nanostructured cathodes provide short diffusion distances, enlarged electrolyte-accessible areas, and open channels that help overcome the strong electrostatic interaction between divalent Zn^{2+} and host lattices. Interlayer expansion, defect engineering, structural water, conductive coatings, and hybridization with carbon can further accelerate Zn^{2+} transport and stabilize repeated insertion and extraction (Blanc *et al.,* 2020; Tang *et al.,* 2024).

The zinc-metal anode nevertheless suffers from non-uniform deposition, dendritic growth, corrosion, passivation, and parasitic hydrogen evolution. Local current-density variations promote protrusions that can penetrate separators, whereas aqueous electrolytes facilitate side reactions and insoluble by-product formation. Cathode degradation may involve dissolution of manganese or vanadium species, irreversible structural transformation, proton co-insertion, and accumulation of basic zinc salts. Three-dimensional zinc hosts, artificial protective layers, electrolyte additives, concentrated electrolytes, and surface-textured current collectors can homogenize Zn^{2+} flux and improve plating-stripping reversibility. Accurate evaluation also requires clarification of the actual charge-storage mechanism because apparent capacity may originate from simultaneous Zn^{2+} insertion, proton participation, conversion reactions, and dissolution-deposition processes (Blanc *et al.,* 2020; Tang *et al.,* 2024).

Metal-air batteries use atmospheric or supplied oxygen as the positive-electrode reactant, reducing the need to store all active cathode material within the cell. In rechargeable zinc-air batteries, zinc is oxidized during discharge while oxygen undergoes the oxygen reduction reaction at a porous air cathode. Charging reverses these processes through zinc deposition and the oxygen evolution reaction. Nanostructured bifunctional catalysts, including heteroatom-doped carbons, metal-nitrogen-carbon materials, spinel oxides, perovskites, layered hydroxides, and hybrid composites, provide abundant active sites and connected transport channels for oxygen, ions, and electrons (Lee *et al.,* 2022).

Metal-air cycling is limited by sluggish oxygen-reduction and oxygen-evolution kinetics, large charge-discharge polarization, catalyst reconstruction, carbon corrosion, electrolyte carbonation, cathode flooding or drying, and pore blockage by discharge products. At the metal electrode, dendrite growth, corrosion, shape change, and passivation further reduce reversibility. Effective air-electrode design therefore requires hierarchical porosity, stable gas-liquid-solid boundaries, corrosion-resistant supports, and catalysts that balance adsorption of oxygen intermediates during both reduction and evolution. For zinc-air batteries, improving the zinc electrode and electrolyte is as important as increasing air-cathode catalytic activity because degradation of either component restricts practical cycle life (Zhang *et al.,* 2019; Lee *et al.,* 2022).

Across lithium-, sodium-, potassium-, zinc-, and metal-air systems, nanomaterials improve ion transport, reaction kinetics, mechanical accommodation, and active-site accessibility. Their practical value, however, depends on controlling interfacial reactivity, particle aggregation, dissolution, phase transformation, and electrode-level density. Future electrode development must integrate nanoscale structural engineering with stable electrolytes, robust binders, conductive networks, protective interphases, and operando characterization. Such integration is necessary to translate high laboratory capacities into rechargeable batteries that retain energy, power, safety, and efficiency over technologically relevant cycling conditions.

6.2. **Nanomaterials for Supercapacitors**

Supercapacitors are electrochemical energy-storage devices distinguished by rapid charge and discharge, high power density, long operational life, and

greater tolerance to repeated cycling than conventional rechargeable batteries. Their performance originates from charge storage at or near the electrode-electrolyte interface rather than from slow, diffusion-limited transformations throughout bulk electrode particles. Nanomaterials are particularly suitable for supercapacitors because their high accessible surface areas, short ion-diffusion distances, tunable pore structures, and abundant redox-active sites can accelerate both ionic and electronic transport. As illustrated in Figure 10, supercapacitor electrodes can operate through electric double-layer capacitance, pseudocapacitance, or battery-type Faradaic reactions, while hybrid configurations combine these mechanisms to balance energy density, power density, response time, and cycling stability (Gogotsi & Penner, 2018; Simon & Gogotsi, 2020).

Electric double-layer capacitors store charge through the reversible electrostatic accumulation of electrolyte ions at the surface of electronically conductive electrodes. Ideally, this mechanism does not involve formal electron transfer across the electrode-electrolyte interface or major crystallographic changes within the active material. Activated carbon, carbon nanotubes, graphene, carbide-derived carbon, carbon aerogels, and biomass-derived porous carbons are therefore widely employed because they combine electrical conductivity, chemical stability, and large internal surface areas. Their cyclic voltammograms are approximately rectangular, while galvanostatic charge-discharge curves are nearly triangular, reflecting rapid and largely non-Faradaic charge storage (Simon & Gogotsi, 2020).

High Brunauer-Emmett-Teller surface area alone does not guarantee high capacitance because only electrolyte-accessible surfaces contribute effectively to charge storage. Micropores can provide high charge-storage density, but pores that are too narrow may restrict ion access or require partial desolvation before ions can enter. Mesopores provide transport pathways and electrolyte reservoirs, while macropores facilitate rapid electrolyte penetration through thick electrodes. Hierarchical pore networks that combine this length scales can therefore improve both capacitance and rate capability. Recent understanding also indicates that nanoscale confinement can produce a continuum between classical double-layer charging and Faradaic storage because ion desolvation, electronic polarization, surface functional groups, and specific ion adsorption modify the interfacial response (Fleischmann *et al.,* 2022; Ge *et al.,* 2025).

Pseudocapacitors store charge through fast and reversible Faradaic processes occurring at or near the electrode surface. These mechanisms include surface redox reactions, reversible ion adsorption accompanied by charge transfer, and intercalation processes that proceed without the slow phase transitions characteristic of conventional battery electrodes. Representative pseudocapacitive materials include RuO_2, MnO_2, NiO, Co_3O_4, Nb_2O_5, MoO_3, transition-metal sulfides, MXenes, and conducting polymers such as polyaniline, polypyrrole, and poly(3,4-ethylenedioxythiophene). Their higher charge-storage density can produce greater specific capacitance than purely carbon-based EDLC electrodes, while their rapid reaction kinetics preserve relatively high-power capability (Choi *et al.,* 2020; Fleischmann *et al.,* 2020).

The distinction between pseudocapacitive and battery-type behaviour must be established kinetically rather than solely from the presence of redox peaks. Pseudocapacitive materials generally exhibit broad electrochemical responses and charge storage that remains rapid across a wide range of current densities. Battery-type materials often display well-defined voltage plateaus associated with diffusion-controlled phase transformations and should preferably be reported using specific capacity in coulombs per gram or milliampere-hours per gram rather than specific capacitance in farads per gram. Figure 10 appropriately differentiates the nearly linear charge-discharge behaviour of capacitive electrodes from the curved response of pseudocapacitive materials and the plateau-containing profile of battery-type electrodes. This distinction is important because converting battery-like capacity into an apparent capacitance can lead to misleading comparisons among electrode systems (Gogotsi & Penner, 2018; Fleischmann *et al.,* 2020).

Hybrid supercapacitors combine materials with complementary charge-storage mechanisms to overcome the limited energy density of EDLCs and the restricted power capability of battery electrodes. Asymmetric supercapacitors commonly pair a positive pseudocapacitive electrode with a negative carbon-based EDLC electrode, whereas battery-supercapacitor hybrids combine a battery-type electrode with a capacitive counterpart. Lithium-ion, sodium-ion, potassium-ion, and zinc-ion hybrid capacitors use ion-insertion or metal-plating reactions at one electrode and rapid interfacial adsorption at the other. Such combinations can broaden the cell-voltage window and increase stored energy, provided that electrode capacities and kinetic responses are appropriately balanced (Choi *et al.,* 2020; Sadavar *et al.,* 2024).

The full-cell schemes in Figure 10 demonstrate how positive and negative electrodes occupy complementary potential ranges, creating a wider operating voltage than either electrode could safely provide alone. Charge balance is essential because an oversized or undersized electrode can force the opposite electrode beyond its stable potential range, accelerating electrolyte decomposition or active-material degradation. Hybrid-cell design must therefore consider the usable capacity, potential window, mass loading, rate capability, and Coulombic efficiency of both electrodes

rather than optimizing each component independently. Conducting polymers are especially promising in hybrid systems because they can exhibit mixed ionic-electronic conductivity, rapid doping and dedoping reactions, mechanical flexibility, and compatibility with carbonaceous or metal-oxide components (Kim & Yoon, 2025).

Conductive networks are central to the electrochemical utilization of nanostructured pseudocapacitive materials. Many transition-metal oxides and hydroxides possess high theoretical charge-storage capacity but low intrinsic electrical conductivity. Integrating them with graphene, carbon nanotubes, carbon nanofibres, MXenes, conductive polymers, or three-dimensional carbon frameworks reduces electron-transport resistance and maintains electrical contact during cycling. These networks can also serve as mechanically resilient scaffolds that prevent nanoparticle aggregation, buffer dimensional changes, and provide interconnected pathways for electrolyte penetration.

Three-dimensional architectures are particularly effective because they integrate electron conduction, ion diffusion, and active-material exposure within the same electrode. Vertically aligned nanosheets, core-shell nanowires, porous aerogels, hollow particles, and binder-free arrays grown directly on conductive substrates can reduce inactive components and minimize interfacial resistance. Nevertheless, excessively dense coatings can block pores, while highly porous electrodes may exhibit low packing density and poor volumetric performance. Restacking of graphene and MXene sheets can further restrict ion access, and oxidation of MXenes or mechanical degradation of conducting polymers may reduce long-term stability. Rational electrode design therefore requires a balance among porosity, conductivity, active-material loading, mechanical strength, and volumetric density.

Specific capacitance is commonly calculated from galvanostatic discharge as $C = I\Delta t/(m\Delta V)$ where I is the discharge current, Δt is the discharge time, m is the relevant active mass, and ΔV is the corrected potential window. Gravimetric capacitance is expressed in F g^{-1}, whereas areal and volumetric capacitances are more appropriate for thin-film, microsupercapacitor, and compact-device applications. Energy density follows approximately $E = \frac{1}{2}C(\Delta V)^2$, demonstrating that increasing the operating voltage is particularly effective because energy varies with the square of voltage. Power density is determined by how rapidly this energy can be delivered and is commonly estimated from the discharge time (Simon & Gogotsi, 2020). These metrics must be reported carefully. Values obtained from a three-electrode configuration characterize an individual electrode and should not be presented as full-device performance. Device-level energy and power densities should include the combined active mass of both electrodes, and practical evaluation should additionally consider current collectors, separators, electrolyte, packaging, electrode thickness, and mass loading. Very high capacitance measured at low active-material loading may decline substantially in thick electrodes because of increased ionic resistance and incomplete utilization. Electrochemical impedance spectroscopy, rate-capability testing, self-discharge analysis, and long-duration cycling are therefore necessary to complement capacitance measurements.

The radar plot in Figure 10 summarizes the central energy-power trade-off. EDLCs provide rapid response, high power, and excellent cycle life but generally lower energy density. Battery-type electrodes provide higher energy but slower kinetics and shorter cycling stability, while pseudocapacitive materials occupy an intermediate region by combining Faradaic charge storage with capacitor-like rates. Nanostructuring shifts this balance by shortening ion-diffusion pathways and exposing more active sites, but it may simultaneously increase side reactions, dissolution, and electrolyte decomposition. Hybrid conductive architectures are consequently required to preserve high-rate transport without sacrificing structural and interfacial stability (Choi *et al.,* 2020; Fleischmann *et al.,* 2020).

Cycling degradation differs among electrode classes. Carbon electrodes may experience electrolyte decomposition, pore blockage, surface oxidation, or loss of electrical contact. Metal oxides and sulfides can undergo dissolution, irreversible phase transformation, agglomeration, or repeated volume changes. Conducting polymers are vulnerable to swelling, contraction, overoxidation, and chain degradation during repeated doping and dedoping. Hybrid nanocomposites can mitigate these processes through mechanical confinement, protective coatings, controlled porosity, and stable conductive scaffolds. Overall, the successful development of nanomaterial-based supercapacitors depends on integrating accessible surface area, rapid redox activity, continuous conductive networks, balanced electrode kinetics, and stable interfaces. Such integration is essential for achieving high specific capacitance and energy density without compromising the defining advantages of high power density and prolonged cycle life.

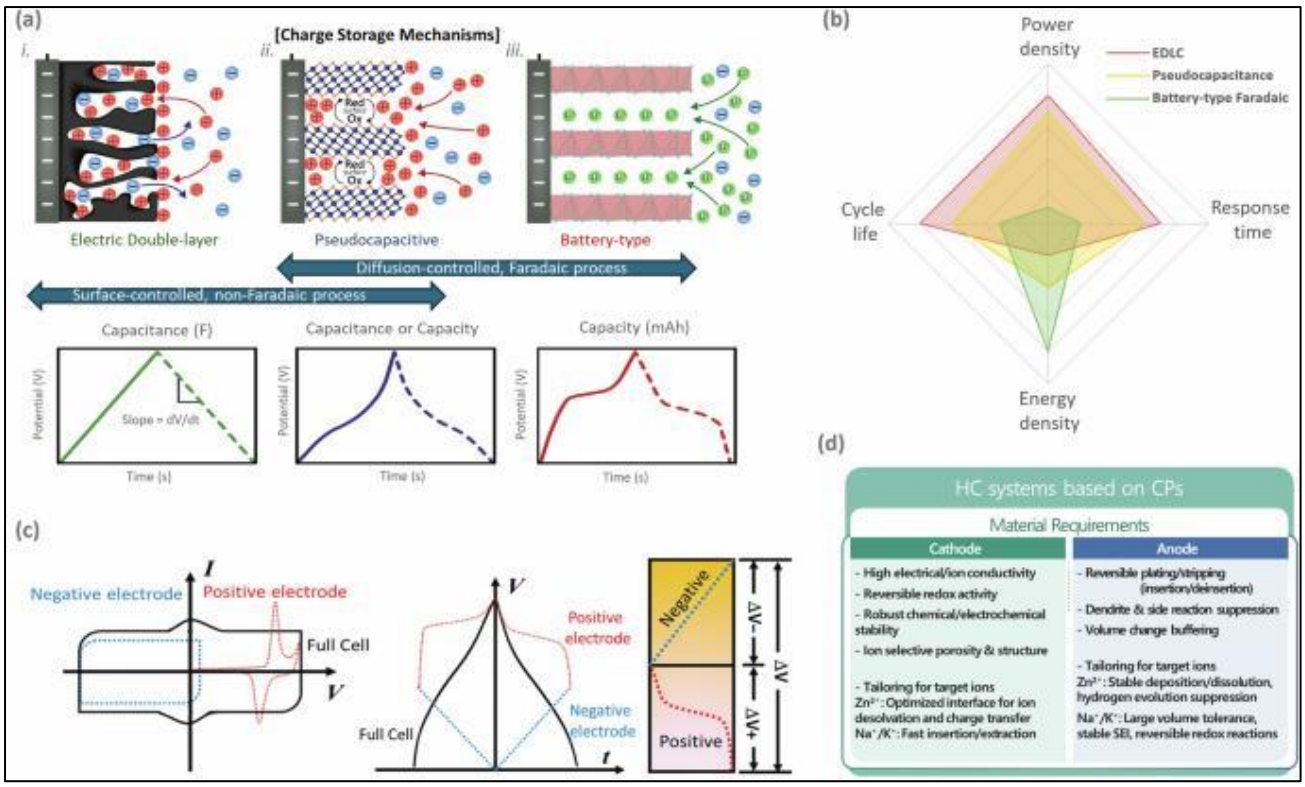

Figure 10: Charge-Storage Mechanisms and Energy-Power Synergy in Nanostructured Supercapacitors

The figure compares electric double-layer, pseudocapacitive, and battery-type Faradaic charge storage together with their characteristic electrochemical responses. It highlights how conductive, high-surface-area hybrid electrodes integrate rapid ion adsorption with reversible redox reactions to improve specific capacitance while balancing energy density, power density, and cycling stability.

6.3. Integrated and Emerging Energy-Storage Systems

Integrated and emerging energy-storage systems extend beyond the optimization of individual electrode materials by combining electrochemical performance with mechanical compliance, structural functionality, device integration, and intelligent energy management. These systems include flexible and wearable batteries, solid-state cells, load-bearing structural batteries, multifunctional electrodes, and hybrid battery–supercapacitor architectures. Nanomaterials are central to these developments because their dimensions, surface chemistry, electrical conductivity, porosity, and mechanical properties can be engineered to support simultaneous ion transport, electron transfer, deformation tolerance, and interfacial stability. However, the increasing complexity of these devices also creates challenges related to durability, safety, manufacturing, performance comparison, and standardization.

Flexible and wearable storage devices must maintain electrochemical performance while undergoing bending, twisting, folding, stretching, and repeated mechanical loading. Conventional battery electrodes are generally deposited on metallic foils that can crack, delaminate, or undergo fatigue during repeated deformation. Flexible systems therefore employ carbon nanotube films, graphene networks, carbon cloth, metal meshes, conducting polymers, hydrogels, and fibrous current collectors as mechanically compliant electronic pathways. Nanowires, nanosheets, porous particles, and interconnected carbon frameworks can accommodate deformation while maintaining contact among active materials, conductive additives, and electrolytes. Gel-polymer and solid-state electrolytes are also used to reduce leakage and preserve ionic conduction under mechanical strain (Riley *et al.,* 2024).

Device architecture is as important as material flexibility. Thin-film batteries provide conformability, fibre-shaped cells can be woven into textiles, and serpentine, kirigami, or origami geometries distribute strain away from electrochemically active regions. Nevertheless, mechanical flexibility cannot be assessed only through photographs of folded devices. Performance should be measured during and after controlled deformation using specified bending radii, tensile strains, loading frequencies, and numbers of mechanical cycles. Electrode cracking, interfacial delamination, separator damage, and loss of electrical contact may develop gradually even when the cell remains visually intact. Ultra-flexible battery design therefore requires simultaneous control of electrochemical interfaces, mechanical neutral planes,

encapsulation, and fatigue-resistant conductive networks (Riley *et al.,* 2024).

Wearable electronics increasingly require autonomous power systems that integrate energy harvesting, conversion, storage, and delivery on the same mechanically compliant platform. Photovoltaic cells, triboelectric and piezoelectric generators, thermoelectric systems, and biofuel cells can be coupled with flexible batteries or supercapacitors to store intermittent energy and provide continuous output. Such integration requires voltage matching, power-management electronics, stable interconnections, and compatible deformation behaviour among all components (Liu *et al.,* 2022). A recent ultra-flexible system combined organic photovoltaic modules with zinc-ion batteries in a device approximately 90 μm thick. The integrated platform achieved a photovoltaic efficiency above 16%, power output exceeding 10 mW cm^{-2}, and areal energy density above 5.82 mWh cm^{-2}, demonstrating the potential of integrated harvesting-storage platforms for wearable sensors and small electronic devices (Saifi *et al.,* 2024).

Solid-state batteries constitute another major emerging storage platform. They replace conventional liquid electrolytes with inorganic ceramic, sulfide, halide, polymeric, or composite solid electrolytes. This configuration can reduce electrolyte leakage and potentially support high-capacity lithium-metal anodes. Solid electrolytes can also provide wide electrochemical stability windows and mechanical barriers against internal short circuits. However, practical performance is controlled by solid-solid interfaces that lack the spontaneous wetting and conformal contact provided by liquids. Poor interfacial contact produces high resistance, nonuniform current distribution, and localized lithium deposition, while chemical reactions between electrodes and electrolytes may generate resistive interphases (Xiao *et al.,* 2020).

Transport through solid-state composite electrodes is also complex because ions must move through a continuous electrolyte network while electrons move through conductive additives and active particles. Insufficient contact, high tortuosity, particle fracture, and loss of percolation can isolate active material during cycling. Volume changes in electrodes generate stress at rigid interfaces, promoting void formation, cracking, delamination, and dendritic penetration. Sulfide electrolytes offer relatively high ionic conductivity and favourable processability but can be chemically sensitive, whereas oxide electrolytes are often mechanically and chemically robust but difficult to densify and integrate with electrodes. Polymers provide better interfacial contact and flexibility but commonly exhibit lower room-temperature conductivity. Composite electrolytes attempt to combine these advantages, although achieving homogeneous dispersion and stable long-term interfaces remains challenging (Janek & Zeier, 2023; Xiao *et al.,* 2020).

Structural batteries integrate energy storage directly into load-bearing components, potentially reducing the mass associated with separate batteries and structural materials. Carbon fibres are particularly attractive because they can function simultaneously as mechanical reinforcement, electronic conductors, current collectors, and lithium-storage electrodes. In a structural battery composite, the electrolyte must conduct ions while transferring mechanical loads between fibres, creating an inherent trade-off between electrochemical transport and stiffness. A structural battery reported by Asp et al. (2021) achieved a specific energy of 24 Wh kg^{-1} together with an elastic modulus of 25 GPa and tensile strength above 300 MPa. Although its energy density remained below that of conventional lithium-ion cells, the combined electrochemical and mechanical functions demonstrate why structural batteries should be evaluated according to multifunctional efficiency rather than energy density alone.

Multifunctional electrodes similarly combine charge storage with additional capabilities such as mechanical reinforcement, strain sensing, self-healing, thermal regulation, energy harvesting, or environmental responsiveness. Carbon nanotubes, graphene, MXenes, conducting polymers, and dynamic polymer networks can provide mixed electronic and ionic conduction while maintaining flexibility. Self-healing binders may reconnect fractured particles, while thermally conductive networks can distribute heat and reduce local temperature gradients. Electrodes may also serve as sensing elements by changing electrical resistance or electrochemical response during deformation. These functions are valuable for wearable electronics and intelligent battery-management systems, but adding multiple components can increase inactive mass, interfacial resistance, processing complexity, and failure probability. Multifunctionality must therefore be demonstrated at the complete-device level rather than inferred from the isolated properties of individual materials (Liu *et al.,* 2022; Riley *et al.,* 2024).

Hybrid battery–supercapacitor systems address the complementary limitations of batteries and electrochemical capacitors. Batteries provide relatively high energy density but may experience polarization, heat generation, and accelerated degradation during rapid power fluctuations. Supercapacitors deliver and accept high power rapidly but store less energy. Connecting the two devices allows the battery to supply average energy demand while the supercapacitor manages short power pulses, regenerative braking, acceleration, and sudden load changes. This division can reduce battery current peaks, temperature rise, and depth-of-discharge fluctuations, potentially extending battery service life (Xu & Shen, 2021).

Hybridization can occur at either the electrochemical cell level or the system level. Hybrid ion

capacitors combine a battery-type Faradaic electrode with a capacitive electrode in one cell, whereas system-level hybrids connect separate batteries and supercapacitors through passive, semi-active, or fully active electrical architectures. Passive configurations are simple but provide limited control over power distribution. Active configurations use bidirectional converters and energy-management algorithms to regulate current and state of charge, although they introduce additional cost, volume, and conversion losses. Electrode kinetics, voltage windows, capacity balance, self-discharge, and ageing rates must be coordinated because mismatch between battery and capacitor components can prevent full utilization of either device. Thus, the effectiveness of hybrid systems depends on both nanomaterial performance and system-level control.

Performance standardization is a major challenge across emerging energy-storage technologies. Material-level values obtained from thin electrodes or three-electrode tests can substantially overestimate practical device performance. Reports should clearly identify whether energy and power densities are calculated using active material, total electrode mass, complete cell mass, or packaged-system mass. Electrode loading, thickness, electrolyte quantity, negative-to-positive capacity ratio, current-collector mass, temperature, voltage range, and cycling protocol should also be specified. Areal and volumetric metrics are particularly important for thin, flexible, and structural devices because high gravimetric values can coexist with low material density or limited total capacity (Noori *et al.,* 2019).

Additional protocols are required for mechanically integrated systems. Flexible devices should report bending radius, strain direction, deformation rate, cycle number, and whether electrochemical testing was conducted during deformation. Structural batteries require simultaneous reporting of energy density, stiffness, strength, damage tolerance, and electrochemical performance under mechanical load. Solid-state battery results are strongly influenced by pellet density, particle size, processing atmosphere, assembly pressure, stack pressure, temperature, and interface preparation. An interlaboratory study involving 21 research groups found considerable variability in all-solid-state cell assembly and cycling despite the use of common materials and a shared electrochemical protocol. The study consequently recommended more complete reporting of assembly parameters and replicate measurements (Puls *et al.,* 2024).

Integrated energy-storage systems therefore require co-design across materials, electrodes, electrolytes, mechanical structures, packaging, and power-management electronics. Nanomaterials can provide conductive, porous, strain-tolerant, and multifunctional frameworks, but their benefits must be demonstrated under realistic mass loadings, deformation conditions, temperatures, and operating times. Progress toward practical implementation will depend on scalable manufacturing, safe interfaces, standardized testing, device-level performance reporting, and evaluation procedures that recognize both electrochemical and non-electrochemical functions.

7. Water Purification and Chemical-Sensing Applications

7.1. Nanomaterial-Based Water Purification Technologies

Nanomaterial-based water purification integrates adsorption, catalytic degradation, membrane separation, antimicrobial treatment, desalination, and interfacial separation within materials possessing high surface areas, tunable pore structures, reactive functional groups, and controllable surface charge. Carbon nanotubes, graphene derivatives, metal and metal-oxide nanoparticles, metal-organic frameworks, porous polymers, nanocellulose, and hybrid nanocomposites can be tailored for selective interactions with inorganic ions, organic molecules, microorganisms, salts, and oil droplets. Their nanoscale dimensions shorten diffusion pathways and increase the density of accessible binding or catalytic sites. However, practical performance depends on selectivity, hydraulic permeability, fouling resistance, regeneration, structural stability, and prevention of nanomaterial release into treated water.

Adsorption is among the most extensively investigated nanomaterial-enabled processes because it can remove contaminants without requiring high pressure or complex reactor systems. Heavy-metal ions are captured through electrostatic attraction, ion exchange, surface complexation, chelation, precipitation, or redox-assisted immobilization. Oxygen-, nitrogen-, sulfur-, and phosphorus-containing groups can coordinate toxic metals such as Pb^{2+}, Cd^{2+}, Hg^{2+}, Cu^{2+}, Ni^{2+}, Cr species, and arsenic oxyanions. Graphene oxide, functionalized carbon nanotubes, iron oxides, layered double hydroxides, biochar nanocomposites, and metal-organic frameworks provide high densities of such binding sites. Nevertheless, adsorption is affected by pH, competing ions, natural organic matter, ionic strength, and contaminant speciation, making performance in real wastewater less predictable than in single-solute laboratory systems (Qasem *et al.,* 2021).

Nanomaterial incorporation into membranes can combine adsorption with physical filtration and simplify adsorbent recovery. Pandey et al. (2022) developed a polyethersulfone membrane containing bis-aminosilane-cross-linked, quaternary-ammonium-functionalized multiwalled carbon nanotubes. The optimized membrane exhibited a pure-water permeability of 312.8 L m^{-2} h^{-1} bar^{-1} and removal efficiencies of approximately 89.5% for Pb^{2+}, 90.4% for Ni^{2+}, 91.4% for Cu^{2+}, and 91.9% for Zn^{2+}. It also retained

substantial permeability and Cu^{2+} rejection after nine treatment cycles. This example demonstrates how nanomaterials can simultaneously modify membrane hydrophilicity, pore architecture, charge, and contaminant affinity, although long-term metal saturation and regeneration remain important considerations.

Dyes and organic contaminants can be captured through pore filling, hydrogen bonding, π-π interactions, hydrophobic inclusion, and electrostatic attraction. Porous carbons and graphene-based adsorbents are effective for aromatic dyes, whereas cyclodextrin polymers, porous organic polymers, and functionalized metal-organic frameworks can provide molecular recognition and size-selective uptake. Alnajrani and Alsager (2020) reported that a polymer of intrinsic microporosity removed at least 80% of doxycycline, ciprofloxacin, penicillin G, and amoxicillin under optimized conditions. Adsorption was attributed to pore filling, electrostatic interactions, aromatic interactions, and hydrogen bonding, illustrating the importance of combining accessible nanoporosity with complementary surface chemistry.

Highly selective porous nanomaterials are also valuable for emerging organic micropollutants present at trace concentrations. Zhang et al. (2021) prepared a magnetic mesoporous nanosponge composed of porous β-cyclodextrin polymers and magnetic nanoparticles. Its hydrophobic cyclodextrin cavities rapidly captured several organic pollutants, achieving approximately 90% removal within about one minute while enabling magnetic separation. Such recoverable adsorbents can reduce post-treatment filtration requirements, but their practical application requires confirmation of performance at environmentally relevant concentrations, in mixed-contaminant matrices, and over repeated adsorption-regeneration cycles.

Photocatalysis provides a destructive treatment pathway rather than merely transferring contaminants to a solid phase. When semiconductor nanoparticles absorb photons with energies sufficient to excite electrons across their bandgap, photogenerated electrons and holes initiate reduction and oxidation reactions. Electrons can reduce dissolved oxygen to superoxide radicals, while holes can directly oxidize adsorbed contaminants or generate hydroxyl radicals from water and hydroxide ions. These reactive species attack dyes, pesticides, pharmaceuticals, antibiotics, endocrine-disrupting chemicals, and other organic micropollutants through hydroxylation, dealkylation, dehalogenation, bond cleavage, and ring-opening reactions.

TiO_2, ZnO, graphitic carbon nitride, bismuth-based semiconductors, and semiconductor-carbon heterostructures are widely investigated photocatalysts. Nanostructuring increases surface reaction sites, while doping, defect engineering, and heterojunction formation can extend light absorption and suppress electron-hole recombination. Nevertheless, disappearance of the parent compound does not necessarily indicate complete mineralization. Photocatalytic studies should therefore evaluate total organic carbon, transformation products, residual toxicity, and catalyst leaching in addition to apparent degradation efficiency.

Immobilizing photocatalysts in membranes improves catalyst recovery and increases contact between contaminants and reactive species. Lotfi et al. (2022) immobilized 10 to 30 nm TiO_2 particles on the surface and within the pores of a polyethersulfone membrane for continuous-flow removal of steroid hormones. At environmentally relevant concentrations, the system removed 80% of both estradiol and estrone under selected operating conditions. Flow through the photocatalytic pores enhanced contact among the micropollutants, catalyst surface, and hydroxyl radicals, demonstrating the potential of photocatalytic membrane reactors for treating trace organic contaminants (Lotfi *et al.,* 2022).

Membrane filtration separates contaminants according to size, charge, solubility, and molecular interactions. Nanomaterial-modified ultrafiltration, nanofiltration, reverse-osmosis, forward-osmosis, and membrane-distillation systems can offer enhanced permeability, selectivity, mechanical strength, and antifouling behaviour. Graphene oxide is particularly attractive because its oxygenated groups promote water affinity, while its stacked nanosheets create adjustable nanochannels for ionic and molecular sieving. However, swelling, delamination, nonuniform stacking, defects, and the conventional permeability-selectivity trade-off remain barriers to reliable desalination and long-term operation (Tiwary *et al.,* 2024).

Rigid nanoparticles can be introduced between two-dimensional sheets to prevent restacking and regulate transport pathways. Zhang et al. (2022) synthesized ultrafine metal oxide-reduced graphene oxide nanocomposites in which sub-3 nm metal-oxide nanoparticles acted as spacers between adjacent sheets. The resulting nanofiltration membranes achieved water permeability of 225 L m^{-2} h^{-1} bar^{-1} and methyl-blue selectivity of up to 98%. This approach demonstrates how nanoparticle spacing can enhance water transport while preserving tortuous pathways required for solute rejection.

For desalination, nanomaterials are incorporated into thin-film composite membranes to increase hydrophilicity, regulate free volume, and provide selective ion-transport channels. Graphene derivatives, zeolites, silica, metal-organic frameworks, aquaporin-inspired channels, and carbon nanotubes are being investigated for reverse osmosis and nanofiltration. Effective desalination requires high salt rejection together with water permeability, chlorine

resistance, mechanical stability, and resistance to organic, inorganic, and biological fouling. Excessive nanoparticle loading can create nonselective voids or aggregation, while some fillers may leach or alter membrane integrity under pressure. Consequently, desalination performance should be evaluated using realistic salinity, cross-flow conditions, prolonged operation, and complete energy-demand analysis.

Renewable nanocomposite membranes may improve the sustainability of pressure-driven filtration. Mir et al. (2024) reinforced bacterial-cellulose membranes with graphene oxide dispersed in poly(ethylene glycol). The optimized composite exhibited nearly twice the water flux and approximately six times the wet compressive strength of pristine bacterial cellulose. It also produced more than 95% flux recovery and rejection of synthetic natural organic matter and bacteria-rich feeds. These results illustrate how nanocellulose and graphene-based materials can combine renewable construction, mechanical reinforcement, pollutant retention, and fouling resistance.

Antimicrobial nanomaterials provide chemical or contact-active control of waterborne pathogens. Silver, copper, ZnO, TiO_2, graphene derivatives, and cationic nanostructures can damage microbial membranes, release toxic metal ions, generate reactive oxygen species, interfere with proteins, or inhibit microbial adhesion. Ghaffari and Sarrafzadeh (2023) modified cellulose filter paper with polydopamine, polyethyleneimine, and a ZnO/Ag/graphene oxide nanocomposite. Three filter layers produced a 99.98% reduction in *Escherichia coli*, while bacterial removal remained above 99.9% after six reuse cycles. The measured zinc and silver concentrations in the filtrate were below the limits considered in that study, highlighting the importance of evaluating antimicrobial efficacy together with nanomaterial leaching.

Oil-water separation is governed mainly by membrane wettability, pore size, surface roughness, and resistance to hydrocarbon fouling. Superhydrophilic and underwater-superoleophobic surfaces allow water to penetrate while repelling oil droplets, whereas superhydrophobic materials may preferentially collect oil from water. Yeh et al. (2023) fabricated a nanopyramidal stainless-steel coating on a cellulose-ester membrane that achieved more than 99% separation of several oil-water emulsions and a maximum permeation flux of 1,555 L m^{-2} h^{-1}. Similarly, Baig and Waheed (2023) developed a PPy@TiO_2/PVDF nanocomposite membrane that maintained oil rejection above 99% and used visible-light photocatalysis to restore surface wettability and permeate flux after fouling. These systems demonstrate the value of integrating separation with self-cleaning functionality.

Despite substantial progress, nanomaterial-enabled purification must be assessed beyond maximum removal percentages. Important criteria include treatment capacity, contact time, pressure demand, catalyst recovery, regeneration chemistry, toxicity, membrane lifetime, nanoparticle release, and performance in real waters. Multifunctional systems that combine adsorption, filtration, photocatalysis, and antimicrobial activity can address mixed contaminants more effectively than single-mechanism materials. Their sustainable implementation, however, will require standardized testing, continuous-flow validation, scalable fabrication, life-cycle assessment, and safe management of contaminant-loaded materials.

7.2. Chemical, Electrochemical, Optical, and Gas Sensors

Nanostructured sensing platforms convert interactions between target analytes and functional materials into measurable electrical, electrochemical, optical, acoustic, piezoelectric, or mass-dependent signals. Their analytical advantages arise from high surface-to-volume ratios, tunable electronic structures, abundant adsorption sites, rapid interfacial charge transfer, and compatibility with miniaturized devices. As illustrated in Figure 11, nanotechnology connects multiple sensing techniques with microfluidics, lab-on-a-chip systems, microelectromechanical devices, and Internet of Things networks for applications spanning environmental monitoring, infectious disease detection, pollution control, and biomedical analysis. Carbon nanomaterials, metallic nanoparticles, metal oxides, quantum dots, MXenes, conducting polymers, and hybrid nanocomposites can therefore serve as both analyte-recognition interfaces and signal-transduction components (Tovar-Lopez, 2023; Darwish *et al.,* 2024).

Chemical sensors generally contain a recognition layer that selectively interacts with an analyte and a transducer that converts this interaction into a quantifiable response. Recognition may occur through adsorption, coordination, electrostatic attraction, redox reactions, catalytic conversion, molecular imprinting, antigen-antibody binding, or aptamer-target association. Nanostructuring increases the proportion of surface atoms available for these interactions and permits functional groups, defects, dopants, and pores to be tailored toward particular targets. However, sensitivity alone is insufficient for reliable analysis because a useful sensor must also possess selectivity, a suitable linear range, low detection and quantification limits, rapid response and recovery, signal stability, reproducibility, and resistance to interference from complex matrices (Darwish *et al.,* 2024).

Electrochemical sensors measure analyte-induced changes in current, potential, impedance, conductivity, or accumulated charge. Amperometric and voltammetric sensors monitor oxidation or reduction currents, potentiometric sensors measure potential

differences under near-zero-current conditions, and impedimetric sensors detect changes in interfacial resistance or capacitance. Nanoparticles and nanostructured carbons increase electroactive surface area, accelerate electron transfer, and provide anchoring sites for enzymes, antibodies, aptamers, or molecularly imprinted polymers. Gold nanoparticles are frequently used because of their conductivity, catalytic activity, and affinity for thiol-containing recognition molecules, whereas graphene, carbon nanotubes, and MXenes establish conductive pathways and support high densities of immobilized receptors (Hara & Singh, 2021; Darwish *et al.,* 2024).

Heavy-metal detection is an important environmental application of electrochemical nanosensors. Ions such as Pb^{2+}, Cd^{2+}, Hg^{2+}, Cu^{2+}, Zn^{2+}, and arsenic species can be accumulated on modified electrodes and quantified through stripping voltammetry, potentiometry, or impedance analysis. Bismuth-based materials, gold nanoparticles, carbon nanostructures, metal-organic frameworks, and MXenes improve metal-ion preconcentration and charge transfer through complexation, electrodeposition, or surface adsorption. Simultaneous detection is possible when different metals generate distinguishable stripping peaks, but overlapping responses, competing ions, variations in pH, and natural organic matter can reduce accuracy. Reliable water analysis therefore requires matrix-specific calibration, recovery testing, and validation against established analytical techniques (Hara & Singh, 2021; Hassan *et al.,* 2022).

Pesticide sensing can employ direct electrochemical oxidation or reduction, catalytic nanomaterial interfaces, or biosensing mechanisms based on enzyme inhibition. Organophosphate and carbamate pesticides are often detected through their inhibition of acetylcholinesterase, which reduces the electrochemical signal produced by enzymatic substrate conversion. Nanostructured metal oxides, gold nanoparticles, carbon nanotubes, graphene, and conducting polymers improve enzyme immobilization and amplify the resulting current change. Non-enzymatic sensors avoid limitations associated with enzyme denaturation and storage, but they may exhibit weaker molecular selectivity. Molecularly imprinted polymers provide an alternative by forming target-shaped recognition cavities, although template removal and nonspecific adsorption must be carefully controlled (Hara & Singh, 2021).

Pharmaceutical residues in environmental and biological samples are increasingly detected using nanomaterial-modified electrochemical electrodes. Antibiotics, anticancer compounds, analgesics, and other drugs may undergo characteristic oxidation or reduction reactions that can be quantified by differential-pulse voltammetry, square-wave voltammetry, or related methods. Carbon nanotubes, graphene derivatives, metallic nanoparticles, metal oxides, and polymer nanocomposites reduce overpotentials and enhance drug-related current responses. Nevertheless, water, serum, urine, and pharmaceutical formulations contain electroactive interferents that may overlap with the target signal. Sensor development must therefore incorporate antifouling coatings, selective receptors, multivariate calibration, and testing in authentic samples rather than relying exclusively on ideal buffer solutions (Qureshi *et al.,* 2024).

Optical nanosensors detect analyte-induced changes in colour, absorbance, fluorescence, luminescence, Raman scattering, or refractive index. Gold and silver nanoparticles are widely used in colorimetric sensing because target-induced aggregation or surface modification changes their localized surface-plasmon resonance and produces a visible colour shift. Quantum dots and carbon dots can exhibit fluorescence enhancement, quenching, wavelength shifts, or lifetime changes following interaction with metal ions, pesticides, pharmaceuticals, and biomolecules. Optical methods can provide rapid and instrument-light detection, but quantitative accuracy may be affected by sample colour, turbidity, photobleaching, particle aggregation, and environmental variations in pH or ionic strength.

Surface-enhanced Raman spectroscopy uses electromagnetic fields generated near nanostructured gold, silver, or hybrid surfaces to amplify the vibrational signatures of adsorbed molecules. This produces chemically informative fingerprints and can support trace-level detection of pesticides, pharmaceutical residues, dyes, pathogens, and volatile compounds. The main limitations are nonuniform enhancement across the substrate, inconsistent hotspot formation, weak adsorption of some targets, and spectral interference from complex samples. Reproducible nanogaps, selective capture layers, microfluidic sample handling, and machine-learning-assisted spectral classification are consequently being developed to improve reliability and multiplexing.

Single-walled carbon nanotubes provide another important class of optical nanosensors because semiconducting nanotubes emit stable near-infrared fluorescence that is sensitive to changes in their local chemical environment. Functional polymers, nucleic acids, peptides, and other surface coatings can impart recognition of proteins, hormones, nucleic acids, pathogens, heavy metals, disinfectants, and small organic molecules. Analyte binding modifies fluorescence intensity or wavelength through changes in surface adsorption, dielectric environment, or exciton behaviour. Near-infrared emission is particularly attractive for biological sensing because it can reduce interference from visible autofluorescence and facilitate measurements in tissues, although nanotube

heterogeneity and functional-coating reproducibility remain important barriers (Dewey *et al.,* 2024).

Gas sensors detect toxic gases and volatile organic compounds through changes in resistance, potential, current, optical absorption, resonance, or mass. Metal-oxide semiconductors such as SnO_2, ZnO, WO_3, In_2O_3, and CuO operate through surface adsorption of oxygen and target gases, which changes carrier concentration and electrical resistance. Nanoparticles, nanowires, hollow spheres, and porous films increase gas-accessible surfaces and shorten diffusion pathways. However, many metal-oxide sensors require elevated temperatures, consume significant power, and show cross-sensitivity to humidity or chemically similar gases.

Two-dimensional materials, particularly graphene derivatives, transition-metal dichalcogenides, and MXenes, provide high conductivity and atomically exposed surfaces that enable room-temperature sensing. MXene surface terminations, defects, interlayer spacing, and oxidation state strongly influence adsorption and charge transfer involving NH_3, NO_2, H_2S, alcohol vapours, acetone, and other volatile compounds. Hybridizing MXenes with metal oxides, graphene, conducting polymers, or transition-metal dichalcogenides can strengthen analyte adsorption and construct heterointerfaces that amplify resistance changes. Practical use remains limited by oxidation, humidity interference, baseline drift, irreversible adsorption, and insufficient selectivity in multicomponent atmospheres (Cai & Kim, 2025).

Gas discrimination can be improved using multisignal sensors and sensor arrays rather than relying on one response from a single material. Zhang et al. (2023) combined chemiresistive and potentiometric outputs to generate multidimensional response patterns for humidity and seven hazardous gases, including ethanol, acetone, toluene, ammonia, carbon monoxide, nitrogen dioxide, and 2-ethylhexanol. Such platforms resemble electronic noses because pattern-recognition algorithms distinguish analytes according to combined response magnitude, dynamics, and recovery behaviour. Machine learning can compensate partly for overlapping selectivity, but models require representative training data covering humidity, temperature, concentration, ageing, and sensor-to-sensor variability (Zhang *et al.,* 2023).

Nanobiosensors extend these principles to biomolecules, microorganisms, and physiological indicators. Enzymes, antibodies, aptamers, nucleic-acid probes, receptors, and molecularly imprinted polymers provide selective recognition of glucose, lactate, hormones, proteins, nucleic acids, pathogens, and therapeutic drugs. Flexible electrodes and soft microfluidic channels allow continuous sampling of sweat, tears, saliva, or interstitial fluid, while electrochemical detection offers low power consumption and compatibility with wearable electronics. Recent sweat-sensing platforms combine nanostructured electrodes with multiplexed detection, microfluidic collection, wireless communication, and energy-harvesting components, although variations in biofluid secretion, contamination, motion, temperature, and individual physiology complicate interpretation (Gao *et al.,* 2023).

For water-quality monitoring, integrated sensor systems can combine electrochemical, optical, and biological channels to detect metals, nutrients, pesticides, pharmaceuticals, microorganisms, and persistent organic contaminants. Emerging targets such as per- and polyfluoroalkyl substances require recognition mechanisms based on fluorophilic, electrostatic, hydrophobic, ion-bridging, or molecular-imprinting interactions. Despite promising laboratory detection limits, real-water performance is often restricted by nonspecific adsorption, low analyte concentrations, dissolved organic matter, salinity, and the presence of structurally related compounds. Consequently, sample enrichment and selective surface chemistry remain necessary for many trace contaminants (Vikesland, 2018; Hassan *et al.,* 2022).

The integration of nanostructured sensors with lab-on-a-chip and Internet of Things technologies, as highlighted in Figure 11, can support automated sampling, multiplexed detection, wireless transmission, and geographically distributed monitoring. Microfluidics reduces sample and reagent consumption and controls transport to the sensing interface, while portable electronics and smartphones enable signal processing outside centralized laboratories. Translation nevertheless requires standardized calibration, batch-to-batch fabrication reproducibility, long-term stability, safe containment of nanomaterials, and validation against regulatory reference methods. Future progress should therefore prioritize selective multifunctional interfaces, antifouling coatings, reference channels, automated quality control, explainable data analysis, and testing under realistic environmental and biological conditions.

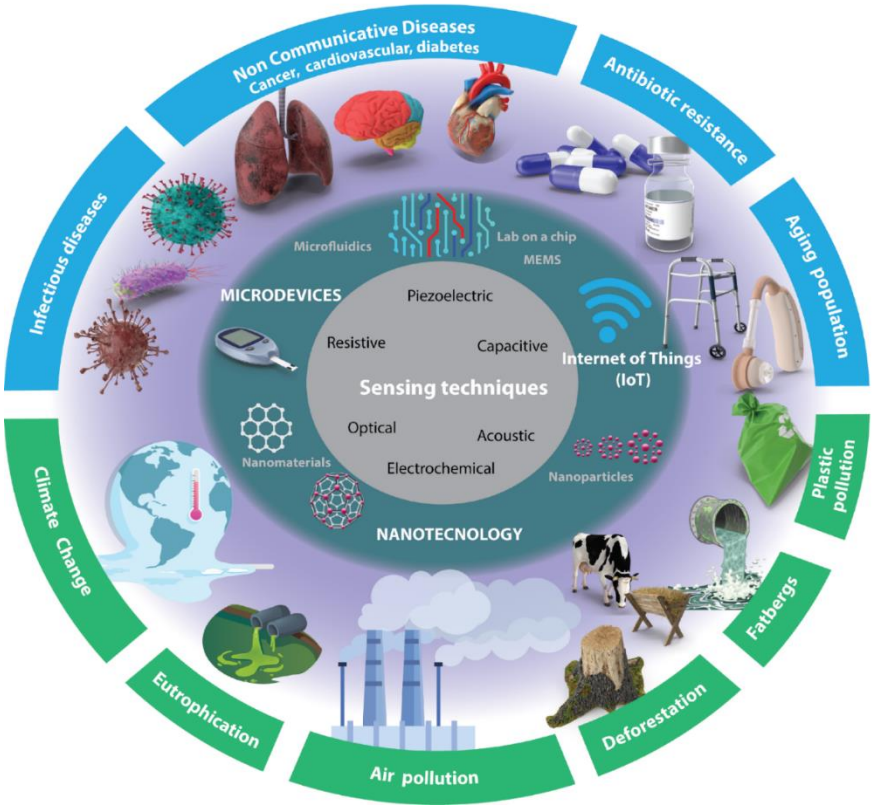

Figure 11: Nanostructured Multimodal Sensors for Chemical, Biological, and Environmental Monitoring

The figure illustrates how nanomaterials, nanoparticles, microfluidics, and miniaturized devices enhance resistive, capacitive, piezoelectric, optical, acoustic, and electrochemical sensing mechanisms. These integrated platforms enable sensitive detection of gaseous pollutants, water contaminants, biomolecules, pharmaceutical compounds, agricultural chemicals, and other environmental hazards, with potential connectivity to real-time Internet of Things monitoring.

7.3. **Integrated Remediation–Sensing Platforms**

Integrated remediation–sensing platforms combine contaminant recognition, quantification, capture, degradation, and treatment verification within a single material or device. Conventional environmental management usually separates laboratory analysis from water treatment, creating delays between pollutant detection and corrective action. Multifunctional nanomaterials can overcome this separation by using the same interfacial properties for both sensing and remediation. Their high surface areas, tunable porosity, catalytic activity, fluorescence, electrical conductivity, and stimulus-responsive behaviour enable pollutants to be detected while they are adsorbed, degraded, filtered, or disinfected. Such integration can support closed-loop treatment in which sensor outputs continuously guide membrane operation, catalyst activation, regeneration, and effluent release.

Smart membranes are among the most promising integrated platforms because they provide a physical separation barrier that can also respond to changes in water chemistry. Stimuli-responsive membranes contain functional polymers, nanoparticles, molecular gates, or conductive layers that alter pore size, wettability, permeability, surface charge, or catalytic activity in response to pH, light, temperature, ionic strength, electric fields, or magnetic fields. These transformations can improve contaminant selectivity, control permeate flux, release accumulated foulants, or activate self-cleaning processes. Photoresponsive membranes may generate reactive oxygen species to degrade adsorbed organics, whereas electrically responsive membranes can regulate ion transport or induce electrochemical oxidation. Magnetic components can assist membrane cleaning or enable remote control of pore structures and surface properties (Mumtaz *et al.,* 2026).

The central advantage of a smart membrane is its capacity to connect treatment performance with environmental conditions. A membrane may remain highly permeable during normal operation but reduce its effective pore size when a target ion or pH change is detected. Similarly, a fouling-related decline in flux could trigger light irradiation, heating, electrical polarization, or mechanical actuation to restore the active surface. However, many reported systems remain proof-of-concept demonstrations because repeated switching can cause polymer fatigue, nanoparticle loss, irreversible pore alteration, or declining responsiveness. Scale-up also requires uniform functionalization across large

membrane areas, low-energy stimulus delivery, and resistance to natural organic matter, salts, microorganisms, and fluctuating wastewater composition.

Self-reporting adsorbents provide a more direct connection between pollutant capture and visual or instrumental detection. These materials generate changes in colour, fluorescence, conductivity, or magnetic response when their binding sites interact with target contaminants. The response can indicate contaminant presence, adsorption progress, or exhaustion of the adsorbent, thereby reducing the need for repeated off-line analysis. Smart adsorbents are commonly based on functional polymers, cellulose, graphene derivatives, metal-organic frameworks, covalent organic frameworks, magnetic nanoparticles, and molecularly imprinted materials. Their recognition mechanisms may involve electrostatic attraction, coordination, ion exchange, hydrophobic interactions, hydrogen bonding, or host-guest inclusion (Nazarzadeh Zare *et al.,* 2021).

A notable example is the cationic TG-PD covalent organic framework developed for simultaneous fluorescent sensing and adsorption of perfluorooctanoic acid. Positively charged guanidinium sites and hydrophobic framework regions promoted selective PFOA binding, while adsorption altered the fluorescence response of the material. The platform exhibited a detection limit of 1.8 μg L^{-1}, rapid uptake, adsorption capacity exceeding 2600 mg g^{-1}, and complete removal at environmentally relevant concentrations in column experiments. This study demonstrates how molecularly engineered porosity can couple recognition and remediation, although extension to complex PFAS mixtures and natural water matrices requires further investigation (Jrad *et al.,* 2024).

Catalytic sensors integrate pollutant detection with chemical transformation. Surface-enhanced Raman scattering substrates are especially suitable because plasmonic nanostructures provide molecular fingerprints at low concentrations, while semiconductor components can photocatalytically degrade the detected compounds. Hu et al. (2020) constructed MoS_2/Fe_2O_3 heterojunction nanocomposites that detected bisphenol A at concentrations as low as 10^{-9} M and subsequently promoted its photocatalytic degradation. Magnetic responsiveness supported material recovery, while photocatalytic cleaning regenerated the sensing surface for reuse. This architecture illustrates how one substrate can identify a contaminant, destroy it, and restore its own sensing capability.

Visible-light-active systems further reduce dependence on ultraviolet irradiation. Wu et al. (2021) developed Au@Cu_2O-Ag nanocomposites that combined strong SERS enhancement with visible-light photocatalytic degradation of malachite green. The plasmonic Ag and Au components amplified Raman signals, while the semiconductor structure supported charge separation and reactive-species generation. More recently, flexible polyimide/TiO_2/Ag microfibres were used for simultaneous SERS detection and photocatalytic degradation of tetracycline. Their flexible architecture facilitated handling and reuse, showing how catalytic sensing can be incorporated into recoverable fibrous devices rather than dispersed nanoparticle suspensions (Han *et al.,* 2024; Wu *et al.,* 2021).

Real-time environmental monitoring requires sensors capable of operating continuously rather than through occasional sample collection. Long-term monitoring systems integrate nanostructured sensing elements with data acquisition, signal processing, wireless transmission, and process control. Electrochemical, optical, resistive, and field-effect sensors can continuously measure parameters such as pH, conductivity, dissolved oxygen, nutrients, metals, organic pollutants, and microbial activity. The resulting data can be analysed using calibration algorithms, anomaly detection, and predictive models to identify contamination events and automatically modify treatment conditions. Continuous monitoring therefore transforms remediation from a fixed process into an adaptive system that responds to temporal and spatial variation in water quality (Huang *et al.,* 2022).

Portable devices extend these capabilities to field-level screening. Paper-based electrochemical strips, smartphone-assisted colorimetric tests, handheld Raman systems, microfluidic chips, and wireless sensor nodes can provide rapid measurements without centralized laboratory infrastructure. Nanomaterials improve portable-device sensitivity by enhancing light absorption, electron transfer, fluorescence, or analyte preconcentration. Integration with smartphones allows image acquisition, calibration, geotagging, and transmission of results to remote databases. Nevertheless, portable systems frequently require sample filtration, pH adjustment, enrichment, or reference measurements to achieve laboratory-level reliability. Battery life, reagent stability, sensor drift, humidity, temperature, and user variability must also be controlled during field deployment (Song *et al.,* 2023).

Active micro- and nanorobots represent an emerging form of mobile remediation-sensing technology. These devices use chemical reactions, magnetic fields, light, ultrasound, or biological propulsion to move through contaminated water, increasing contact with pollutants beyond diffusion-controlled limits. Functional microrobots can capture heavy metals, plastics, oils, organic contaminants, and microorganisms while carrying electrochemical or optical recognition components. Magnetic or phototactic guidance can support targeted treatment and subsequent recovery. However, practical deployment requires biocompatible propulsion, reliable retrieval, scalable manufacturing, collective motion control, and prevention

of secondary contamination from the robotic materials themselves (Urso *et al.,* 2023).

Regeneration is essential because integrated platforms are economically and environmentally valuable only when sensing and remediation functions can be restored without major material loss. Adsorbents may be regenerated through pH adjustment, salt washing, solvent extraction, thermal treatment, or competitive desorption. Photocatalytic self-cleaning can mineralize adsorbed organic molecules, while magnetic recovery can simplify separation from treated water. Regeneration protocols must preserve pore structure, recognition sites, catalytic activity, and calibration accuracy. A platform may retain adsorption capacity while losing fluorescence intensity or electrochemical sensitivity, meaning that both treatment and sensing functions must be evaluated after each cycle.

Selectivity remains a major challenge because environmental samples contain competing ions, natural organic matter, suspended particles, salts, and structurally related contaminants. High affinity alone does not guarantee selective recognition, especially when nonspecific fouling changes optical or electrical signals. Molecular imprinting, aptamers, host-guest cavities, ion-selective ligands, and size-controlled porous frameworks can improve discrimination. Multisensor arrays and pattern-recognition algorithms provide an alternative by identifying contaminants from combined response profiles rather than a single selective interaction. However, algorithmic classification must be trained using realistic mixtures and environmental conditions to prevent overestimated performance.

Field-level validation should therefore include continuous-flow operation, realistic contaminant concentrations, mixed matrices, seasonal variation, mechanical stress, regeneration, and independent comparison with standardized analytical methods. Key metrics should include detection limit, treatment capacity, response time, recovery, selectivity, flux, energy consumption, material leaching, signal drift, false-positive rate, and operational lifetime. Integrated remediation–sensing platforms offer a pathway toward autonomous environmental treatment, but successful implementation will require durable materials, standardized testing, recoverable nanostructures, reliable data interpretation, and demonstrated performance beyond controlled laboratory solutions.

8. CONCLUSION

Advanced multifunctional nanomaterials have emerged as versatile platforms for addressing interconnected challenges in sustainable energy, environmental remediation, water purification, and chemical sensing. Their significance arises from the ability to integrate multiple functions within a single material system, including catalytic activity, light harvesting, ion storage, electrical conductivity, molecular recognition, selective adsorption, antimicrobial action, and responsive interfacial behaviour. These capabilities allow nanomaterials to perform tasks that conventional single-function materials cannot achieve efficiently, such as simultaneously detecting, capturing, and degrading pollutants or combining energy storage with mechanical, sensing, and structural functions. The performance of multifunctional nanomaterials is governed by complex relationships among composition, dimensionality, morphology, crystallinity, porosity, defects, surface chemistry, and interfacial electronic structure. Nanoscale features such as vacancies, dopants, low-coordination atoms, exposed crystal facets, heterojunctions, and metal-support interfaces can regulate adsorption strength, charge separation, ion diffusion, redox kinetics, and product selectivity. Therefore, rational design must extend beyond increasing surface area and instead focus on controlling the identity, accessibility, stability, and dynamics of active sites under operating conditions. Advanced microscopy, spectroscopy, electrochemical analysis, and in situ or operando characterization are essential for identifying these working structures and connecting material properties with real-time performance.

Green synthesis and sustainable fabrication provide important routes for reducing the environmental burden of nanomaterial production. Biological precursors, renewable biomolecules, waste-derived feedstocks, mechanochemical processing, microwave-assisted methods, and low-temperature synthesis can reduce hazardous reagent use and energy consumption. However, sustainability must be evaluated across the complete material life cycle, including precursor sourcing, solvent demand, purification, scalability, recovery, regeneration, recyclability, and end-of-life management. A synthesis route should not be considered environmentally favourable solely because it uses a biological reducing agent or renewable precursor.

In catalytic and photocatalytic applications, multifunctional nanomaterials can accelerate chemical reactions, improve solar-fuel generation, and promote the degradation of persistent pollutants. Their effectiveness depends on balanced adsorption and desorption, suitable band-edge positions, efficient charge-carrier separation, controlled reactive-species formation, selective surface reactions, and resistance to photocorrosion or structural transformation. For environmental remediation, degradation of a parent contaminant should not be treated as equivalent to complete detoxification. Mineralization, transformation-product identification, residual toxicity, catalyst recovery, and reusability must be evaluated to confirm genuine treatment effectiveness. Nanostructured electrodes have also expanded the capabilities of rechargeable batteries, supercapacitors, and emerging integrated energy-storage systems. Their short diffusion pathways, high interfacial area, conductive networks,

and strain-accommodating architectures can improve capacity, rate performance, and mechanical flexibility. Nevertheless, excessive surface reactivity may accelerate electrolyte decomposition, interphase growth, dissolution, and structural degradation. Future energy-storage research must therefore balance nanoscale kinetic advantages with electrode density, interfacial stability, safety, complete-device performance, and long-term cycling. Flexible devices, solid-state batteries, structural batteries, and hybrid battery-supercapacitor systems further require standardized mechanical and electrochemical testing under realistic operating conditions.

In water purification, nanomaterials enable adsorption, photocatalysis, membrane filtration, desalination, antimicrobial treatment, and oil-water separation. Their high surface areas and tailored functional groups allow effective removal of heavy metals, dyes, pharmaceuticals, pesticides, pathogens, oils, and organic micropollutants. The integration of sensing and remediation offers an especially promising pathway toward autonomous treatment systems. Smart membranes, self-reporting adsorbents, catalytic sensors, microfluidic devices, and Internet of Things-connected platforms can identify contamination, initiate treatment, monitor performance, and indicate when regeneration is required. Their practical success will depend on selectivity, antifouling behaviour, calibration stability, material recovery, low energy demand, and validation in real environmental matrices.

The major barriers to sustainable implementation include toxicity, aggregation, instability, leaching, limited selectivity, difficult recovery, inconsistent reproducibility, high production cost, and insufficient standardization. Many laboratory studies continue to rely on simplified conditions, low material loadings, single-contaminant solutions, short cycling periods, or idealized test systems. Future investigations should prioritize continuous-flow operation, realistic pollutant concentrations, complex matrices, long-term durability, regeneration, complete mass balances, life-cycle assessment, and techno-economic evaluation.

Artificial intelligence, machine learning, autonomous experimentation, and high-throughput screening can accelerate the discovery and optimization of multifunctional nanomaterials. These tools can help identify promising compositions, predict structure-property-performance relationships, optimize synthesis conditions, and interpret complex operando datasets. However, computational predictions must be supported by mechanistic understanding, reproducible experiments, standardized testing, and independent validation. Overall, multifunctional nanomaterials offer a powerful foundation for next-generation technologies in clean energy, water security, environmental protection, and real-time chemical monitoring. Their transition from laboratory demonstrations to practical systems will require coordinated progress in sustainable synthesis, surface and interface engineering, device integration, safety assessment, circular design, standardization, and scalable manufacturing. By adopting safe-by-design, circular-by-design, and systems-level development strategies, these materials can contribute meaningfully to efficient, economical, and environmentally responsible energy and environmental technologies.

REFERENCES

- Abraham, K. M. (2020). How comparable are sodium-ion batteries to lithium-ion counterparts? *ACS Energy Letters, 5*(11), 3544–3547. DOI: 10.1021/acsenergylett.0c02181
- Ahmed, M. A., Mahmoud, S. A., & Mohamed, A. A. (2025). Interfacially engineered metal oxide nanocomposites for enhanced photocatalytic degradation of pollutants and energy applications. *RSC Advances, 15*, 15561–15603. DOI: 10.1039/D4RA08780A
- Alnajrani, M. N., & Alsager, O. A. (2020). Removal of antibiotics from water by polymer of intrinsic microporosity: Isotherms, kinetics, thermodynamics, and adsorption mechanism. *Scientific Reports, 10*, Article 794. DOI: 10.1038/s41598-020-57616-4
- Asp, L. E., Bouton, K., Carlstedt, D., Duan, S., Harnden, R., Johannisson, W., Johansen, M., Johansson, M. K. G., Lindbergh, G., Liu, F., Peuvot, K., Schneider, L. M., Xu, J., & Zenkert, D. (2021). A structural battery and its multifunctional performance. *Advanced Energy and Sustainability Research, 2*(3), Article 2000093. DOI: 10.1002/aesr.202000093
- Baek, J., Hossain, M. D., Mukherjee, P., Lee, J., Winther, K. T., Leem, J., Jiang, Y., Chueh, W. C., Bajdich, M., & Zheng, X. (2023). Synergistic effects of mixing and strain in high entropy spinel oxides for oxygen evolution reaction. *Nature Communications, 14*, Article 5936. DOI: 10.1038/s41467-023-41359-7
- Baig, N., Kammakakam, I., & Falath, W. (2021). Nanomaterials: A review of synthesis methods, properties, recent progress, and challenges. *Materials Advances, 2*(6), 1821–1871. DOI: 10.1039/D0MA00807A
- Baig, U., & Waheed, A. (2023). A facile strategy for fabrication of nanocomposite ultrafiltration membrane: Oily wastewater treatment and photocatalytic self-cleaning. *npj Clean Water, 6*, Article 68. DOI: 10.1038/s41545-023-00279-1
- Barrera, L., & Bala Chandran, R. (2021). Harnessing photoelectrochemistry for wastewater nitrate treatment coupled with resource recovery. *ACS Sustainable Chemistry & Engineering, 9*(10), 3688–3701. DOI: 10.1021/acssuschemeng.0c07935
- Bennett, T. D., Coudert, F.-X., James, S. L., & Cooper, A. I. (2021). The changing state of porous

materials. *Nature Materials, 20*, 1179–1187. DOI: 10.1038/s41563-021-00957-w

- Bhattacharjee, K., & Prasad, B. L. V. (2023). Surface functionalization of inorganic nanoparticles with ligands: A necessary step for their utility. *Chemical Society Reviews, 52*, 2573–2595. DOI: 10.1039/D1CS00876E
- Blanc, L. E., Kundu, D., & Nazar, L. F. (2020). Scientific challenges for the implementation of Zn-ion batteries. *Joule, 4*(4), 771–799. DOI: 10.1016/j.joule.2020.03.002
- Cai, Z., & Kim, H. (2025). Recent advances in MXene gas sensors: Synthesis, composites, and mechanisms. *npj 2D Materials and Applications, 9*, Article 66. DOI: 10.1038/s41699-025-00586-w
- Checa, M., Fuhr, A. S., Sun, C., Vasudevan, R., Ziatdinov, M., Ivanov, I., Yun, S. J., Xiao, K., Sehirlioglu, A., Kim, Y., Sharma, P., Kelley, K. P., Domingo, N., Jesse, S., & Collins, L. (2023). High-speed mapping of surface charge dynamics using sparse scanning Kelvin probe force microscopy. *Nature Communications, 14*, Article 7196. DOI: 10.1038/s41467-023-42583-x
- Chen, D., Cheng, Y., Zhou, N., Chen, P., Wang, Y., Li, K., Huo, S., Cheng, P., Peng, P., Zhang, R., Wang, L., Liu, H., Liu, Y., & Ruan, R. (2020). Photocatalytic degradation of organic pollutants using TiO_2-based photocatalysts: A review. *Journal of Cleaner Production, 268*, Article 121725. DOI: 10.1016/j.jclepro.2020.121725
- Choi, C., Ashby, D. S., Butts, D. M., DeBlock, R. H., Wei, Q., Lau, J., & Dunn, B. (2020). Achieving high energy density and high power density with pseudocapacitive materials. *Nature Reviews Materials, 5*(1), 5–19. DOI: 10.1038/s41578-019-0142-z
- Darwish, M. A., Abd-Elaziem, W., Elsheikh, A., & Zayed, A. A. (2024). Advancements in nanomaterials for nanosensors: A comprehensive review. *Nanoscale Advances, 6*(16), 4015–4046. DOI: 10.1039/D4NA00214H
- De Silva, M., Cao, G., & Tam, K. C. (2025). Nanomaterials for the removal and detection of heavy metals: A review. *Environmental Science: Nano, 12*, 2154–2191. DOI: 10.1039/D4EN01041H
- Deng, X., Zhang, J., Qi, K., Liang, G., Xu, F., & Yu, J. (2024). Ultrafast electron transfer at the In_2O_3/Nb_2O_5 S-scheme interface for CO_2 photoreduction. *Nature Communications, 15*, Article 4807. DOI: 10.1038/s41467-024-49004-7
- Dewey, H. M., Lamb, A., & Budhathoki-Uprety, J. (2024). Recent advances on applications of single-walled carbon nanotubes as cutting-edge optical nanosensors for biosensing technologies. *Nanoscale, 16*(35), 16344–16375. DOI: 10.1039/D4NR01892C
- Edge, J. S., O'Kane, S., Prosser, R., Kirkaldy, N. D., Patel, A. N., Hales, A., Ghosh, A., Ai, W., Chen, J., Yang, J., Li, S., Pang, M.-C., Bravo Diaz, L., Tomaszewska, A., Marzook, M. W., Radhakrishnan, K. N., Wang, H., Patel, Y., Wu, B., & Offer, G. J. (2021). Lithium ion battery degradation: What you need to know. *Physical Chemistry Chemical Physics, 23*(14), 8200–8221. DOI: 10.1039/D1CP00359C
- Efros, A. L., & Brus, L. E. (2021). Nanocrystal quantum dots: From discovery to modern development. *ACS Nano, 15*(4), 6192–6210. DOI: 10.1021/acsnano.1c01399
- Fleischmann, S., Mitchell, J. B., Wang, R., Zhan, C., Jiang, D. E., Presser, V., & Augustyn, V. (2020). Pseudocapacitance: From fundamental understanding to high power energy storage materials. *Chemical Reviews, 120*(14), 6738–6782. DOI: 10.1021/acs.chemrev.0c00170
- Fleischmann, S., Zhang, Y., Wang, X., Cummings, P. T., Wu, J., Simon, P., Gogotsi, Y., Presser, V., & Augustyn, V. (2022). Continuous transition from double-layer to Faradaic charge storage in confined electrolytes. *Nature Energy, 7*(3), 222–228. DOI: 10.1038/s41560-022-00993-z
- Gahlawat, G., & Choudhury, A. R. (2019). A review on the biosynthesis of metal and metal salt nanoparticles by microbes. *RSC Advances, 9*(23), 12944–12967. DOI: 10.1039/C8RA10483B
- Gao, F., Liu, C., Zhang, L., Liu, T., Wang, Z., Song, Z., Cai, H., Fang, Z., Chen, J., Wang, J., Han, M., Wang, J., Lin, K., Wang, R., Li, M., Mei, Q., Ma, X., Liang, S., Gou, G., & Xue, N. (2023). Wearable and flexible electrochemical sensors for sweat analysis: A review. *Microsystems & Nanoengineering, 9*, Article 1. DOI: 10.1038/s41378-022-00443-6
- Ge, K., Shao, H., Lin, Z., Taberna, P. L., & Simon, P. (2025). Advanced characterization of confined electrochemical interfaces in electrochemical capacitors. *Nature Nanotechnology, 20*(2), 196–208. DOI: 10.1038/s41565-024-01821-z
- Ge, S., Wei, K., Peng, W., Huang, R., Akinlabi, E., Xia, H., Shahzad, M. W., Zhang, X., Xu, B. B., & Jiang, J. (2024). A comprehensive review of covalent organic frameworks (COFs) and their derivatives in environmental pollution control. *Chemical Society Reviews, 53*(23), 11259–11302. DOI: 10.1039/D4CS00521J
- Ghaffari, S.-B., & Sarrafzadeh, M.-H. (2023). Cationic cellulose filter papers modified with ZnO/Ag/GO nanocomposite as point-of-use gravity-driven filters for bacterial removal from water. *Scientific Reports, 13*, Article 22604. DOI: 10.1038/s41598-023-50114-3
- Giansante, C. (2020). Library design of ligands at the surface of colloidal nanocrystals. *Accounts of Chemical Research, 53*(8), 1458–1467. DOI: 10.1021/acs.accounts.0c00204
- Gogotsi, Y., & Penner, R. M. (2018). Energy storage in nanomaterials: Capacitive, pseudocapacitive, or

battery-like? *ACS Nano, 12*(3), 2081–2083. DOI: 10.1021/acsnano.8b01914

- Gong, E., Ali, S., Hiragond, C. B., Kim, H. S., Powar, N. S., Kim, D., Kim, H., & In, S.-I. (2022). Solar fuels: Research and development strategies to accelerate photocatalytic CO_2 conversion into hydrocarbon fuels. *Energy & Environmental Science, 15*, 880–937. DOI: 10.1039/D1EE02714J
- Gonzalez-Gallardo, C. L., Arjona, N., Álvarez-Contreras, L., & Guerra-Balcázar, M. (2022). Electrochemical creatinine detection for advanced point-of-care sensing devices: A review. *RSC Advances, 12*(47), 30785–30802. DOI: 10.1039/D2RA04479J
- Gopinath, K. P., Madhav, N. V., Krishnan, A., Malolan, R., & Rangarajan, G. (2020). Present applications of titanium dioxide for the photocatalytic removal of pollutants from water: A review. *Journal of Environmental Management, 270*, Article 110906. DOI: 10.1016/j.jenvman.2020.110906
- Grimaldi, F., Pucciarelli, M., Gavriilidis, A., Dobson, P., & Lettieri, P. (2020). Anticipatory life cycle assessment of gold nanoparticles production: Comparison of milli-continuous flow and batch synthesis. *Journal of Cleaner Production, 269*, Article 122335. DOI: 10.1016/j.jclepro.2020.122335
- Guilger-Casagrande, M., & de Lima, R. (2019). Synthesis of silver nanoparticles mediated by fungi: A review. *Frontiers in Bioengineering and Biotechnology, 7*, Article 287. DOI: 10.3389/fbioe.2019.00287
- Guo, Y., Bae, J., Fang, Z., Li, P., Zhao, F., & Yu, G. (2020). Hydrogels and hydrogel-derived materials for energy and water sustainability. *Chemical Reviews, 120*(15), 7642–7707. DOI: 10.1021/acs.chemrev.0c00345
- Han, D., Guo, B., Li, Y., Feng, W., Liu, K., Wu, T., Wan, Y., Wang, L., Gao, M., Liu, Y., Yang, L., Wei, M., & Yang, S. (2024). Simultaneous photocatalytic degradation and SERS detection of tetracycline with self-sustainable and recyclable ternary PI/TiO_2/Ag flexible microfibers. *Microsystems & Nanoengineering, 10*, Article 39. DOI: 10.1038/s41378-023-00624-x
- Hara, T. O., & Singh, B. (2021). Electrochemical biosensors for detection of pesticides and heavy metal toxicants in water: Recent trends and progress. *ACS ES&T Water, 1*(3), 462–478. DOI: 10.1021/acsestwater.0c00125
- Hassan, M. H., Khan, R., & Andreescu, S. (2022). Advances in electrochemical detection methods for measuring contaminants of emerging concerns. *Electrochemical Science Advances, 2*(6), Article e2100184. DOI: 10.1002/elsa.202100184
- Hessel, V., Tran, N. N., Asrami, M. R., Tran, Q. D., Long, N. V. D., Escribà-Gelonch, M., Tejada, J. O., Linke, S., & Sundmacher, K. (2022). Sustainability of green solvents: Review and perspective. *Green Chemistry, 24*(2), 410–437. DOI: 10.1039/D1GC03662A
- Hosaka, T., Kubota, K., Hameed, A. S., & Komaba, S. (2020). Research development on K-ion batteries. *Chemical Reviews, 120*(14), 6358–6466. DOI: 10.1021/acs.chemrev.9b00463
- Hu, M., Quan, Y., Yang, S., Su, R., Liu, H., Gao, M., Chen, L., & Yang, J. (2020). Self-cleaning semiconductor heterojunction substrate: Ultrasensitive detection and photocatalytic degradation of organic pollutants for environmental remediation. *Microsystems & Nanoengineering, 6*, Article 111. DOI: 10.1038/s41378-020-00222-1
- Huang, K., Hu, C., Tan, Q., Wu, S., Shabala, S., Yu, M., & Sun, X. (2025). Nanozymes as a tool to boost agricultural production: From preparation to application. *Environmental Science: Nano, 12*(1), 98–120. DOI: 10.1039/D4EN00780H
- Huang, Y., Wang, X., Xiang, W., Wang, T., Otis, C., Sarge, L., Lei, Y., & Li, B. (2022). Forward-looking roadmaps for long-term continuous water quality monitoring: Bottlenecks, innovations, and prospects in a critical review. *Environmental Science & Technology, 56*(9), 5334–5354. DOI: 10.1021/acs.est.1c07857
- Hughes, K. J., Iyer, K. A., Bird, R. E., Ivanov, J., Banerjee, S., Georges, G., & Zhou, Q. A. (2024). Review of carbon nanotube research and development: Materials and emerging applications. *ACS Applied Nano Materials, 7*(16), 18695–18713. DOI: 10.1021/acsanm.4c02721
- Isaacs, M. A., Davies-Jones, J., Davies, P. R., Guan, S., Lee, R., Morgan, D. J., & Palgrave, R. (2021). Advanced XPS characterization: XPS-based multi-technique analyses for comprehensive understanding of functional materials. *Materials Chemistry Frontiers, 5*, 7931-7963. DOI: 10.1039/D1QM00969A
- Janek, J., & Zeier, W. G. (2023). Challenges in speeding up solid-state battery development. *Nature Energy, 8*, 230–240. DOI: 10.1038/s41560-023-01208-9
- Jeevanandam, J., Barhoum, A., Chan, Y. S., Dufresne, A., & Danquah, M. K. (2018). Review on nanoparticles and nanostructured materials: History, sources, toxicity and regulations. *Beilstein Journal of Nanotechnology, 9*, 1050–1074. DOI: 10.3762/bjnano.9.98
- Jrad, A., Das, G., Alkhatib, N., Prakasam, T., Benyettou, F., Varghese, S., Gándara, F., Olson, M., Kirmizialtin, S., & Trabolsi, A. (2024). Cationic covalent organic framework for the fluorescent sensing and cooperative adsorption of perfluorooctanoic acid. *Nature Communications, 15*, Article 10490. DOI: 10.1038/s41467-024-53945-4
- Kang, S., Rahman, A., McGinnis, S., & Vikesland, P. (2024). Toward environmentally favorable nano-

sensing by production of reusable gold nanoparticles from gold nano-waste: Life cycle and nanocircular economy implications. *Environmental Science: Nano, 11*, 1499–1507. DOI: 10.1039/D3EN00505D

- Kang, S., Rahman, A., McGinnis, S., & Vikesland, P. (2024). Toward environmentally favorable nano-sensing by production of reusable gold nanoparticles from gold nano-waste: Life cycle and nanocircular economy implications. *Environmental Science: Nano, 11*, 1499–1507. DOI: 10.1039/D3EN00505D
- Khan, I., Saeed, K., & Khan, I. (2019). Nanoparticles: Properties, applications and toxicities. *Arabian Journal of Chemistry, 12*(7), 908–931. DOI: 10.1016/j.arabjc.2017.05.011
- Khan, S., Noor, T., Iqbal, N., & Yaqoob, L. (2024). Photocatalytic dye degradation from textile wastewater: A review. *ACS Omega, 9*(20), 21751–21767. DOI: 10.1021/acsomega.4c00887
- Khosravi, A., Zarepour, A., Iravani, S., Varma, R. S., & Zarrabi, A. (2024). Sustainable synthesis: Natural processes shaping the nanocircular economy. *Environmental Science: Nano, 11*, 688–707. DOI: 10.1039/D3EN00973D
- Kiani, D., & Wachs, I. E. (2024a). The conundrum of "pair sites" in Langmuir-Hinshelwood reaction kinetics in heterogeneous catalysis. *ACS Catalysis, 14*(13), 10260–10270. DOI: 10.1021/acscatal.4c02813
- Kiani, D., & Wachs, I. E. (2024b). Practical considerations for understanding surface reaction mechanisms involved in heterogeneous catalysis. *ACS Catalysis, 14*(22), 16770–16784. DOI: 10.1021/acscatal.4c05188
- Kim, M., Goerzen, D., Jena, P. V., Zeng, E., Pasquali, M., Meidl, R. A., & Heller, D. A. (2024). Human and environmental safety of carbon nanotubes across their life cycle. *Nature Reviews Materials, 9*(1), 63–81. DOI: 10.1038/s41578-023-00611-8
- Kim, S., & Yoon, H. (2025). The strategic role of conducting polymers in zinc- and alkali-ion hybrid capacitors. *Communications Materials, 6*, Article 278. DOI: 10.1038/s43246-025-01008-6
- Koe, W. S., Lee, J. W., Chong, W. C., Pang, Y. L., & Sim, L. C. (2020). An overview of photocatalytic degradation: Photocatalysts, mechanisms, and development of photocatalytic membrane. *Environmental Science and Pollution Research, 27*, 2522–2565. DOI: 10.1007/s11356-019-07193-5
- Lee, S., Choi, J., Kim, M., Park, J., Park, M., & Cho, J. (2022). Material design and surface chemistry for advanced rechargeable zinc-air batteries. *Chemical Science, 13*, 6159–6180. DOI: 10.1039/D1SC07212A
- Leybo, D., Etim, U. J., Monai, M., Bare, S. R., Zhong, Z., & Vogt, C. (2024). Metal-support interactions in metal oxide-supported atomic, cluster, and nanoparticle catalysis. *Chemical Society Reviews, 53*, 10450-10490. DOI: 10.1039/D4CS00527A
- Li, C., Liu, J., Li, H., Wu, K., Wang, J., & Yang, Q. (2022). Covalent organic frameworks with high quantum efficiency in sacrificial photocatalytic hydrogen evolution. *Nature Communications, 13*, Article 2357. DOI: 10.1038/s41467-022-30035-x
- Li, W., Zhou, T., Zhang, Z., Li, L., Lian, W., Wang, Y., Lu, J., Yan, J., Wang, H., Wei, L., & Cheng, Q. (2024). Ultrastrong MXene film induced by sequential bridging with liquid metal. *Science, 385*(6704), 62–68. DOI: 10.1126/science.ado4257
- Li, Z., Ji, S., Liu, Y., Cao, X., Tian, S., Chen, Y., Niu, Z., & Li, Y. (2020). Well-defined materials for heterogeneous catalysis: From nanoparticles to isolated single-atom sites. *Chemical Reviews, 120*(2), 623–682. DOI: 10.1021/acs.chemrev.9b00311
- Lin, L., Ma, Y., Vequizo, J. J. M., Nakabayashi, M., Gu, C., Tao, X., Yoshida, H., Pihosh, Y., Nishina, Y., Yamakata, A., Shibata, N., Hisatomi, T., Takata, T., & Domen, K. (2024). Efficient and stable visible-light-driven Z-scheme overall water splitting using an oxysulfide H_2 evolution photocatalyst. *Nature Communications, 15*, Article 397. DOI: 10.1038/s41467-024-44706-4
- Ling, F., Kang, W., Jing, H., Zeng, W., Chen, Y., Liu, X., Zhang, Y., Qi, L., Fang, L., & Zhou, M. (2019). Enhancing hydrogen evolution on the basal plane of transition metal dichalcogenide van der Waals heterostructures. *npj Computational Materials, 5*, Article 20. DOI: 10.1038/s41524-019-0161-8
- Liu, L., & Corma, A. (2018). Metal catalysts for heterogeneous catalysis: From single atoms to nanoclusters and nanoparticles. *Chemical Reviews, 118*(10), 4981–5079. DOI: 10.1021/acs.chemrev.7b00776
- Liu, L., Meira, D. M., Arenal, R., Concepción, P., Puga, A. V., & Corma, A. (2019). Determination of the evolution of heterogeneous single metal atoms and nanoclusters under reaction conditions: Which are the working catalytic sites? *ACS Catalysis, 9*(12), 10626–10639. DOI: 10.1021/acscatal.9b04214
- Liu, R., Wang, Z. L., Fukuda, K., & Someya, T. (2022). Flexible self-charging power sources. *Nature Reviews Materials, 7*, 870–886. DOI: 10.1038/s41578-022-00441-0
- Lotfi, S., Fischer, K., Schulze, A., & Schäfer, A. I. (2022). Photocatalytic degradation of steroid hormone micropollutants by TiO_2-coated polyethersulfone membranes in a continuous flow-through process. *Nature Nanotechnology, 17*, 417–423. DOI: 10.1038/s41565-022-01074-8
- Lu, L., Zou, S., & Fang, B. (2021). The critical impacts of ligands on heterogeneous nanocatalysis: A review. *ACS Catalysis, 11*(10), 6020–6058. DOI: 10.1021/acscatal.1c00903

- Lu, X., Chen, Z., Chen, G., & Liu, Z. (2024). Metal–organic framework based self-powered devices for human body energy harvesting. *Chemical Communications, 60*(61), 7843–7865. DOI: 10.1039/D4CC02110J
- Lu, Y., Cai, Y., Zhang, S., Zhuang, L., Hu, B., Wang, S., Chen, J., & Wang, X. (2022). Application of biochar-based photocatalysts for adsorption-(photo)degradation/reduction of environmental contaminants: Mechanism, challenges and perspective. *Biochar, 4*, Article 45. DOI: 10.1007/s42773-022-00173-y
- Luo, J., Zhang, S., Sun, M., Yang, L., Luo, S., & Crittenden, J. C. (2019). A critical review on energy conversion and environmental remediation of photocatalysts with remodeling crystal lattice, surface, and interface. *ACS Nano, 13*(9), 9811–9840. DOI: 10.1021/acsnano.9b03649
- Ma, Y., Yi, X., Wang, S., Li, T., Tan, B., Chen, C., Majima, T., Waclawik, E. R., Zhu, H., & Wang, J. (2022). Selective photocatalytic CO_2 reduction in aerobic environment by microporous Pd-porphyrin-based polymers coated hollow TiO_2. *Nature Communications, 13*, Article 1400. DOI: 10.1038/s41467-022-29102-0
- Manthiram, A. (2020). A reflection on lithium-ion battery cathode chemistry. *Nature Communications, 11*, Article 1550. DOI: 10.1038/s41467-020-15355-0
- Mir, I. S., Riaz, A., Fréchette, J., Roy, J. S., Mcelhinney, J., Pu, S., Balakrishnan, H. K., Greener, J., Dumée, L. F., & Messaddeq, Y. (2024). Bacterial cellulose-graphene oxide composite membranes with enhanced fouling resistance for bio-effluents management. *npj Clean Water, 7*, Article 111. DOI: 10.1038/s41545-024-00403-9
- Mitchell, S., Qin, R., Zheng, N., & Pérez-Ramírez, J. (2021). Nanoscale engineering of catalytic materials for sustainable technologies. *Nature Nanotechnology, 16*(2), 129–139. DOI: 10.1038/s41565-020-00799-8
- Modi, S., Shah, Y., Okonkwo, O., Gilbertson, L. M., & Biswas, P. (2025). Toward sustainable scaled-up synthesis of lignin-derived carbon nanoparticles using a furnace aerosol reactor: Insights from a life cycle assessment. *Environmental Science & Technology, 59*(37), 19802–19812. DOI: 10.1021/acs.est.5c06572
- Mourdikoudis, S., Pallares, R. M., & Thanh, N. T. K. (2018). Characterization techniques for nanoparticles: Comparison and complementarity upon studying nanoparticle properties. *Nanoscale, 10*(27), 12871-12934. DOI: 10.1039/C8NR02278J
- Muhammad, P., Zada, A., Rashid, J., Hanif, S., Gao, Y., Li, C., Li, Y., Fan, K., & Wang, Y. (2024). Defect engineering in nanocatalysts: From design and synthesis to applications. *Advanced Functional Materials, 34*(29), Article 2314686. DOI: 10.1002/adfm.202314686
- Mumtaz, F., Faraz, M., Balakrishnan, H. K., Nair, R., & Dumée, L. F. (2026). Stimuli-responsive membranes: Mechanisms, materials and future directions. *npj Clean Water, 9*, Article 1. DOI: 10.1038/s41545-025-00533-8
- Nagar, A., & Pradeep, T. (2020). Clean water through nanotechnology: Needs, gaps, and fulfillment. *ACS Nano, 14*(6), 6420–6435. DOI: 10.1021/acsnano.9b01730
- Nazari, M., Zadehahmadi, F., Sadiq, M. M., Sutton, A. L., Mahdavi, H., & Hill, M. R. (2024). Challenges and solutions to the scale-up of porous materials. *Communications Materials, 5*, Article 170. DOI: 10.1038/s43246-024-00608-y
- Nazarzadeh Zare, E., Mudhoo, A., Ali Khan, M., Otero, M., Bundhoo, Z. M. A., Patel, M., Srivastava, A., Navarathna, C., Mlsna, T., Mohan, D., Pittman, C. U., Jr., Makvandi, P., & Sillanpää, M. (2021). Smart adsorbents for aquatic environmental remediation. *Small, 17*(34), Article 2007840. DOI: 10.1002/smll.202007840
- Nishiyama, H., Yamada, T., Nakabayashi, M., Maehara, Y., Yamaguchi, M., Kuromiya, Y., Nagatsuma, Y., Tokudome, H., Akiyama, S., Watanabe, T., Narushima, R., Okunaka, S., Shibata, N., Takata, T., Hisatomi, T., & Domen, K. (2021). Photocatalytic solar hydrogen production from water on a 100-m² scale. *Nature, 598*, 304–307. DOI: 10.1038/s41586-021-03907-3
- Noori, A., El-Kady, M. F., Rahmanifar, M. S., Kaner, R. B., & Mousavi, M. F. (2019). Towards establishing standard performance metrics for batteries, supercapacitors and beyond. *Chemical Society Reviews, 48*(5), 1272–1341. DOI: 10.1039/C8CS00581H
- Österberg, M., Henn, K. A., Farooq, M., & Valle-Delgado, J. J. (2023). Biobased nanomaterials: The role of interfacial interactions for advanced materials. *Chemical Reviews, 123*(5), 2200–2241. DOI: 10.1021/acs.chemrev.2c00492
- Osterrieth, J. W. M., Rampersad, J., Madden, D., Rampal, N., Skoric, L., Connolly, B., Allendorf, M. D., Stavila, V., Snider, J. L., Ameloot, R., Marreiros, J., Ania, C., Azevedo, D., Vilarrasa-Garcia, E., Santos, B. F., Bu, X.-H., Chang, Z., Bunzen, H., Champness, N. R., ... Fairen-Jimenez, D. (2022). How reproducible are surface areas calculated from the BET equation? *Advanced Materials, 34*(27), Article 2201502. DOI: 10.1002/adma.202201502
- Pandey, R. P., Ouda, M., Rasheed, P. A., Banat, F., & Hasan, S. W. (2022). Surface decoration of bis-aminosilane cross-linked multiwall carbon nanotube ultrafiltration membrane for fast and efficient heavy metal removal. *npj Clean Water, 5*, Article 44. DOI: 10.1038/s41545-022-00189-8
- Patiño-Ruiz, D. A., Meramo-Hurtado, S. I., González-Delgado, Á. D., & Herrera, A. (2021). Environmental sustainability evaluation of iron oxide nanoparticles synthesized via green synthesis

and the coprecipitation method: A comparative life cycle assessment study. *ACS Omega, 6*(19), 12410–12423. DOI: 10.1021/acsomega.0c05246

- Patiño-Ruiz, D. A., Meramo-Hurtado, S. I., González-Delgado, Á. D., & Herrera, A. (2021). Environmental sustainability evaluation of iron oxide nanoparticles synthesized via green synthesis and the coprecipitation method: A comparative life cycle assessment study. *ACS Omega, 6*(19), 12410–12423. DOI: 10.1021/acsomega.0c05246
- Pervez, M. N., Balakrishnan, M., Hasan, S. W., Choo, K.-H., Zhao, Y., Cai, Y., Zarra, T., Belgiorno, V., & Naddeo, V. (2020). A critical review on nanomaterials membrane bioreactor for wastewater treatment. *npj Clean Water, 3*, Article 43. DOI: 10.1038/s41545-020-00090-2
- Pilling, R., Coles, S. R., Knecht, M. R., & Patwardhan, S. V. (2023). Multi-criteria discovery, design and manufacturing to realise nanomaterial potential. *Communications Engineering, 2*, Article 78. DOI: 10.1038/s44172-023-00128-6
- Pokrajac, L., Abbas, A., Chrzanowski, W., Dias, G. M., Eggleton, B. J., Maguire, S., Maine, E., Malloy, T., Nathwani, J., Nazar, L., Sips, A., Sone, J., van den Berg, A., Weiss, P. S., & Mitra, S. K. (2021). Nanotechnology for a sustainable future: Addressing global challenges with the International Network4Sustainable Nanotechnology. *ACS Nano, 15*(12), 18608–18623. DOI: 10.1021/acsnano.1c10919
- Pomerantseva, E., Bonaccorso, F., Feng, X., Cui, Y., & Gogotsi, Y. (2019). Energy storage: The future enabled by nanomaterials. *Science, 366*(6468), eaan8285. DOI: 10.1126/science.aan8285
- Popovic, J. (2021). The importance of electrode interfaces and interphases for rechargeable metal batteries. *Nature Communications, 12*, Article 6240. DOI: 10.1038/s41467-021-26481-8
- Prajapati, A., Hahn, C., Weidinger, I. M., Shi, Y., Lee, Y., Alexandrova, A. N., Thompson, D., Bare, S. R., Chen, S., Yan, S., & Kornienko, N. (2025). Best practices for in-situ and operando techniques within electrocatalytic systems. *Nature Communications, 16*, Article 2593. DOI: 10.1038/s41467-025-57563-6
- Puls, S., Nazmutdinova, E., Kalyk, F., Woolley, H. M., Thomsen, J. F., Cheng, Z., Fauchier-Magnan, A., Gautam, A., Gockeln, M., Ham, S.-Y., Hasan, M. T., Jeong, M.-G., Hiraoka, D., Kim, J. S., Kutsch, T., Lelotte, B., Minnmann, P., Miß, V., Motohashi, K., ... Vargas-Barbosa, N. M. (2024). Benchmarking the reproducibility of all-solid-state battery cell performance. *Nature Energy, 9*(10), 1310–1320. DOI: 10.1038/s41560-024-01634-3
- Qasem, N. A. A., Mohammed, R. H., & Lawal, D. U. (2021). Removal of heavy metal ions from wastewater: A comprehensive and critical review. *npj Clean Water, 4*, Article 36. DOI: 10.1038/s41545-021-00127-0
- Qureshi, A., Shah, A., Iftikhar, F. J., Haleem, A., & Zia, M. A. (2024). Electrochemical analysis of anticancer and antibiotic drugs in water and biological specimens. *RSC Advances, 14*(49), 36633–36655. DOI: 10.1039/D4RA05685J
- Rajaitha, P. M., Hajra, S., Mistewicz, K., Panda, S., Sahu, M., Dubal, D., Yamauchi, Y., & Kim, H. J. (2022). Multifunctional materials for photo-electrochemical water splitting. *Journal of Materials Chemistry A, 10*(30), 15906–15931. DOI: 10.1039/D2TA01869A
- Rangarajan, G., Jayaseelan, A., & Farnood, R. (2022). Photocatalytic reactive oxygen species generation and their mechanisms of action in pollutant removal with biochar supported photocatalysts: A review. *Journal of Cleaner Production, 346*, Article 131155. DOI: 10.1016/j.jclepro.2022.131155
- Rani, A., Snyder, S. W., Kim, H., Lei, Z., & Pan, S.-Y. (2022). Pathways to a net-zero-carbon water sector through energy-extracting wastewater technologies. *npj Clean Water, 5*, Article 49. DOI: 10.1038/s41545-022-00197-8
- Rawlings, A. E., Somner, L. A., Fitzpatrick-Milton, M., Roebuck, T. P., Gwyn, C., Liravi, P., Seville, V., Neal, T. J., Mykhaylyk, O. O., Baldwin, S. A., & Staniland, S. S. (2019). Artificial coiled coil biomineralisation protein for the synthesis of magnetic nanoparticles. *Nature Communications, 10*, Article 2873. DOI: 10.1038/s41467-019-10578-2
- Ren, Y., Fu, Y., Li, N., You, C., Huang, J., Huang, K., Sun, Z., Zhou, J., Si, Y., Zhu, Y., Chen, W., Duan, L., & Liu, M. (2024). Concentrated solar CO_2 reduction in H_2O vapour with >1% energy conversion efficiency. *Nature Communications, 15*, Article 4675. DOI: 10.1038/s41467-024-49003-8
- Riley, S., Shevchuk, A., & George, C. (2024). Achieving dynamic stability and electromechanical resilience for ultra-flexible battery technology. *Communications Materials, 5*, Article 268. DOI: 10.1038/s43246-024-00703-0
- Sadavar, S. V., Lee, S. Y., & Park, S. J. (2024). Advancements in asymmetric supercapacitors: From historical milestones to challenges and future directions. *Advanced Science, 11*, Article 2403172. DOI: 10.1002/advs.202403172
- Saifi, S., Xiao, X., Cheng, S., Guo, H., Zhang, J., Müller-Buschbaum, P., Zhou, G., Xu, X., & Cheng, H.-M. (2024). An ultraflexible energy harvesting-storage system for wearable applications. *Nature Communications, 15*, Article 6546. DOI: 10.1038/s41467-024-50894-w
- Sarma, B. B., Maurer, F., Doronkin, D. E., & Grunwaldt, J. D. (2023). Design of single-atom catalysts and tracking their fate using operando and advanced X-ray spectroscopic tools. *Chemical Reviews, 123*(1), 379–444. DOI: 10.1021/acs.chemrev.2c00495

- Sayed, M., Qi, K., Wu, X., Zhang, L., García, H., & Yu, J. (2025). Cu-based S-scheme photocatalysts. *Chemical Society Reviews, 54*, 4874-4921. DOI: 10.1039/D4CS01091D
- Sharma, N. K., Vishwakarma, J., Rai, S., Alomar, T. S., AlMasoud, N., & Bhattarai, A. (2022). Green route synthesis and characterization techniques of silver nanoparticles and their biological adeptness. *ACS Omega, 7*(31), 27004–27020. DOI: 10.1021/acsomega.2c01400
- Simon, P., & Gogotsi, Y. (2020). Perspectives for electrochemical capacitors and related devices. *Nature Materials, 19*(11), 1151–1163. DOI: 10.1038/s41563-020-0747-z
- Singh, S., Sivaram, N., Nath, B., Khan, N. A., Singh, J., & Ramamurthy, P. C. (2024). Metal organic frameworks for wastewater treatment, renewable energy and circular economy contributions. *npj Clean Water, 7*, Article 124. DOI: 10.1038/s41545-024-00408-4
- Song, H. W., Choi, W., Jeon, T., & Oh, J. H. (2023). Recent advances in smart organic sensors for environmental monitoring systems. *ACS Applied Electronic Materials, 5*(1), 77–99. DOI: 10.1021/acsaelm.2c01315
- Srivastava, S. K. (2024). Recent advances in removal of pharmaceutical pollutants in wastewater using metal oxides and carbonaceous materials as photocatalysts: A review. *RSC Applied Interfaces, 1*, 340–429. DOI: 10.1039/D3LF00142C
- Su, H., Pan, X., Li, S., Zhang, H., & Zou, R. (2023). Defect-engineered two-dimensional transition metal dichalcogenides towards electrocatalytic hydrogen evolution reaction. *Carbon Energy, 5*, Article e296. DOI: 10.1002/cey2.296
- Subhiksha, V., Kokilavani, S., & Sudheer Khan, S. (2022). Recent advances in degradation of organic pollutant in aqueous solutions using bismuth based photocatalysts: A review. *Chemosphere, 290*, Article 133228. DOI: 10.1016/j.chemosphere.2021.133228
- Sun, Y., Li, C., Liu, D., Zhang, F., Xue, J., & Zheng, Q. (2025). Surface and interfacial engineering for multifunctional nanocarbon materials. *ACS Nano, 19*(2), 1944–1980. DOI: 10.1021/acsnano.4c14128
- Takata, T., Jiang, J., Sakata, Y., Nakabayashi, M., Shibata, N., Nandal, V., Seki, K., Hisatomi, T., & Domen, K. (2020). Photocatalytic water splitting with a quantum efficiency of almost unity. *Nature, 581*, 411–414. DOI: 10.1038/s41586-020-2278-9
- Tang, L., Peng, H., Kang, J., Chen, H., Zhang, M., Liu, Y., Kim, D. H., Liu, Y., & Lin, Z. (2024). Zn-based batteries for sustainable energy storage: Strategies and mechanisms. *Chemical Society Reviews, 53*, 4877–4925. DOI: 10.1039/D3CS00295K
- Tarannum, N., Divya, & Gautam, Y. K. (2019). Facile green synthesis and applications of silver nanoparticles: A state-of-the-art review. *RSC Advances, 9*(60), 34926–34948. DOI: 10.1039/C9RA04164H
- Tariq, S. R., Niaz, Z., Chotana, G. A., Ahmad, D., & Rafique, N. (2023). Photocatalytic degradation of imidacloprid using Ag_2O/CuO composites. *RSC Advances, 13*, 19326–19334. DOI: 10.1039/D3RA02109B
- Tiwary, S. K., Singh, M., Chavan, S. V., & Karim, A. (2024). Graphene oxide-based membranes for water desalination and purification. *npj 2D Materials and Applications, 8*, Article 27. DOI: 10.1038/s41699-024-00462-z
- Tovar-Lopez, F. J. (2023). Recent progress in micro- and nanotechnology-enabled sensors for biomedical and environmental challenges. *Sensors, 23*(12), Article 5406. DOI: 10.3390/s23125406
- Urso, M., Ussia, M., & Pumera, M. (2023). Smart micro- and nanorobots for water purification. *Nature Reviews Bioengineering, 1*, 236–251. DOI: 10.1038/s44222-023-00025-9
- VahidMohammadi, A., Rosen, J., & Gogotsi, Y. (2021). The world of two-dimensional carbides and nitrides (MXenes). *Science, 372*(6547), eabf1581. DOI: 10.1126/science.abf1581
- van Deelen, T. W., Hernández Mejía, C., & de Jong, K. P. (2019). Control of metal-support interactions in heterogeneous catalysts to enhance activity and selectivity. *Nature Catalysis, 2*(11), 955–970. DOI: 10.1038/s41929-019-0364-x
- Vigil, T. N., & Spangler, L. C. (2024). Understanding biomineralization mechanisms to produce size-controlled, tailored nanocrystals for optoelectronic and catalytic applications: A review. *ACS Applied Nano Materials, 7*(16), 18626–18654. DOI: 10.1021/acsanm.3c04277
- Vikesland, P. J. (2018). Nanosensors for water quality monitoring. *Nature Nanotechnology, 13*(8), 651–660. DOI: 10.1038/s41565-018-0209-9
- Vogt, C., & Weckhuysen, B. M. (2022). The concept of active site in heterogeneous catalysis. *Nature Reviews Chemistry, 6*(2), 89–111. DOI: 10.1038/s41570-021-00340-y
- Wan, S., Li, X., Chen, Y., Liu, N., Du, Y., Dou, S., Jiang, L., & Cheng, Q. (2021). High-strength scalable MXene films through bridging-induced densification. *Science, 374*(6563), 96–99. DOI: 10.1126/science.abg2026
- Wan, S., Wang, W., Cheng, B., Luo, G., Shen, Q., Yu, J., Zhang, J., Cao, S., & Zhang, L. (2024). A superlattice interface and S-scheme heterojunction for ultrafast charge separation and transfer in photocatalytic H_2 evolution. *Nature Communications, 15*, Article 9612. DOI: 10.1038/s41467-024-53951-6
- Wang, A., Chen, Y., Zheng, Z., Wang, H., Li, X., Yang, Z., Qiu, R., & Yan, K. (2021). In situ N-doped carbon-coated mulberry-like cobalt manganese oxide boosting for visible light driving photocatalytic degradation of pharmaceutical

pollutants. *Chemical Engineering Journal, 411*, Article 128497. DOI: 10.1016/j.cej.2021.128497

- Wang, H., Shao, Y., Mei, S., Lu, Y., Zhang, M., Sun, J.-K., Matyjaszewski, K., Antonietti, M., & Yuan, J. (2020). Polymer-derived heteroatom-doped porous carbon materials. *Chemical Reviews, 120*(17), 9363–9419. DOI: 10.1021/acs.chemrev.0c00080
- Wang, J., Hsu, C.-S., Wu, T.-S., Chan, T.-S., Suen, N.-T., Lee, J.-F., & Chen, H. M. (2023). In situ X-ray spectroscopies beyond conventional X-ray absorption spectroscopy on deciphering dynamic configuration of electrocatalysts. *Nature Communications, 14*, Article 6576. DOI: 10.1038/s41467-023-42370-8
- Wang, S., Zhang, J., Gharbi, O., Vivier, V., Gao, M., & Orazem, M. E. (2021). Electrochemical impedance spectroscopy. *Nature Reviews Methods Primers, 1*, Article 41. DOI: 10.1038/s43586-021-00039-w
- Wang, X., Wang, X., Huang, J., Li, S., Meng, A., & Li, Z. (2021). Interfacial chemical bond and internal electric field modulated Z-scheme S_v-$ZnIn_2S_4$/$MoSe_2$ photocatalyst for efficient hydrogen evolution. *Nature Communications, 12*, Article 4112. DOI: 10.1038/s41467-021-24511-z
- Wang, X., Wu, J., Zhang, Y., Sun, Y., Ma, K., Xie, Y., Zheng, W., Tian, Z., Kang, Z., & Zhang, Y. (2023). Vacancy defects in 2D transition metal dichalcogenide electrocatalysts: From aggregated to atomic configuration. *Advanced Materials, 35*(50), Article 2206576. DOI: 10.1002/adma.202206576
- Wang, Y., Wei, J.-X., Tang, H.-L., Shao, L.-H., Dong, L.-Z., Chu, X.-Y., Jiang, Y.-X., Zhang, G.-L., Zhang, F.-M., & Lan, Y.-Q. (2024). Artificial photosynthetic system for diluted CO_2 reduction in gas-solid phase. *Nature Communications, 15*, Article 8818. DOI: 10.1038/s41467-024-53066-y
- Wang, Z., Xue, N., & Chen, J. (2019). Semiconductor-cocatalyst interfacial electron transfer dominates photocatalytic reaction. *The Journal of Physical Chemistry C, 123*(40), 24404-24408. DOI: 10.1021/acs.jpcc.9b06698
- Wu, T., Zheng, H., Kou, Y., et al. (2021). Self-sustainable and recyclable ternary Au@Cu_2O-Ag nanocomposites: Application in ultrasensitive SERS detection and highly efficient photocatalysis of organic dyes under visible light. *Microsystems & Nanoengineering, 7*, Article 23. DOI: 10.1038/s41378-021-00250-5
- Xiao, Y., Wang, Y., Bo, S.-H., Kim, J. C., Miara, L. J., & Ceder, G. (2020). Understanding interface stability in solid-state batteries. *Nature Reviews Materials, 5*(2), 105–126. DOI: 10.1038/s41578-019-0157-5
- Xu, H., & Shen, M. (2021). The control of lithium-ion batteries and supercapacitors in hybrid energy storage systems for electric vehicles: A review. *International Journal of Energy Research, 45*(15), 20524–20544. DOI: 10.1002/er.7150
- Xu, J., Shao, G., Tang, X., Lv, F., Xiang, H., Jing, C., Liu, S., Dai, S., Li, Y., Luo, J., & Zhou, Z. (2022). Frenkel-defected monolayer MoS_2 catalysts for efficient hydrogen evolution. *Nature Communications, 13*, Article 2193. DOI: 10.1038/s41467-022-29929-7
- Yan, Q.-Q., Wu, D.-X., Chu, S.-Q., Chen, Z.-Q., Lin, Y., Chen, M.-X., Zhang, J., Wu, X.-J., & Liang, H.-W. (2019). Reversing the charge transfer between platinum and sulfur-doped carbon support for electrocatalytic hydrogen evolution. *Nature Communications, 10*, Article 4977. DOI: 10.1038/s41467-019-12851-w
- Yang, H., Zhang, G.-X., Zhou, H.-J., Sun, Y.-Y., & Pang, H. (2023). Metal–organic frameworks meet MXene: New opportunities for electrochemical application. *Energy Material Advances, 4*, Article 0033. DOI: 10.34133/energymatadv.0033
- Yeh, Y.-J., Chu, J. P., You, J.-D., Chang, T.-H., Liou, J. R., Chiang, W.-H., Yiu, P., Hsueh, C.-H., Shen, Y.-L., & Tung, K.-L. (2023). Tunable nanostructured stainless-steel coating for high-selective and high-permeable separation membranes for oil/water emulsions. *npj Clean Water, 6*, Article 17. DOI: 10.1038/s41545-023-00237-x
- Zachman, M. J., Fung, V., Polo-Garzon, F., Cao, S., Moon, J., Huang, Z., Jiang, D.-E., Wu, Z., & Chi, M. (2022). Measuring and directing charge transfer in heterogenous catalysts. *Nature Communications, 13*, Article 3253. DOI: 10.1038/s41467-022-30923-2
- Zhai, P., Xia, M., Wu, Y., Zhang, G., Gao, J., Zhang, B., Cao, S., Zhang, Y., Li, Z., Fan, Z., Wang, C., Zhang, X., Miller, J. T., Sun, L., & Hou, J. (2021). Engineering single-atomic ruthenium catalytic sites on defective nickel-iron layered double hydroxide for overall water splitting. *Nature Communications, 12*, Article 4587. DOI: 10.1038/s41467-021-24828-9
- Zhai, P., Zhang, Y., Wu, Y., Gao, J., Zhang, B., Cao, S., Zhang, Y., Li, Z., Sun, L., & Hou, J. (2020). Engineering active sites on hierarchical transition bimetal oxides/sulfides heterostructure array enabling robust overall water splitting. *Nature Communications, 11*, Article 5462. DOI: 10.1038/s41467-020-19214-w
- Zhang, H., Zhang, Z., Li, Z., Han, H., Song, W., & Yi, J. (2023). A chemiresistive-potentiometric multivariate sensor for discriminative gas detection. *Nature Communications, 14*, Article 3495. DOI: 10.1038/s41467-023-39213-x
- Zhang, J., Zhou, Q., Tang, Y., Zhang, L., & Li, Y. (2019). Zinc-air batteries: Are they ready for prime time? *Chemical Science, 10*, 8924–8929. DOI: 10.1039/C9SC04221K
- Zhang, L., Guo, Y., Hao, R., Shi, Y., You, H., Nan, H., Dai, Y., Liu, D., Lei, D., & Fang, J. (2021). Ultra-rapid and highly efficient enrichment of organic pollutants via magnetic mesoporous

nanosponge for ultrasensitive nanosensors. *Nature Communications, 12*, Article 6849. DOI: 10.1038/s41467-021-27100-2

- Zhang, P., Hu, Y., Yao, B., Guo, J., Ye, Z., & Peng, X. (2024). Metal-organic frameworks for solar-driven desalination. *Communications Materials, 5*, Article 92. DOI: 10.1038/s43246-024-00534-z
- Zhang, W., Xu, H., Xie, F., Ma, X., Niu, B., Chen, M., Zhang, H., Zhang, Y., & Long, D. (2022). General synthesis of ultrafine metal oxide/reduced graphene oxide nanocomposites for ultrahigh-flux nanofiltration membrane. *Nature Communications, 13*, Article 471. DOI: 10.1038/s41467-022-28180-4
- Zhao, Y., Tong, T., Wang, X., Lin, S., Reid, E. M., & Chen, Y. (2021). Differentiating solutes with precise nanofiltration for next-generation environmental separations: A review. *Environmental Science & Technology, 55*(3), 1359–1376. DOI: 10.1021/acs.est.0c04593
- Zheng, Z., He, J., Zhang, Z., Kumar, A., Khan, M., Lung, C. W., & Lo, I. M. C. (2024). Magnetically recyclable nanophotocatalysts in photocatalysis-involving processes for organic pollutant removal from wastewater: Current status and perspectives. *Environmental Science: Nano, 11*, 1784–1816. DOI: 10.1039/D3EN00906H